

# ALL Detailed Program of Accepted Minisymposia

**TOC of part\_1**

**TOC of part\_2**

**[00023] Recent advances on application driven nonlinear optimization**

- [01318] A Unified Single-loop Alternating Gradient Projection Algorithm for Nonconvex-Concave and Convex-Nonconcave Minimax Problems
- [01287] Accelerated ADMM-type Methods for Convex and Nonconvex Optimization Problems
- [01284] On a special discrete phase constrained complex-field optimization problem
- [01368] Stochastic regularized Newton methods for nonlinear equations
- [01475] An Efficient Quadratic-Programming Relaxation Based Algorithm for Large-Scale MIMO Detection
- [01487] Uniform Framework of Convergence Analysis for Nesterov's Accelerated Gradient Method
- [01285] Exact continuous relaxations and algorithms for regularized optimization problems

**[00024] Geometric methods in machine learning and data analysis**

- [03148] Geometric Data Analysis via Discrete Curvature
- [02978] Large data limit of the MBO scheme for data clustering
- [03210] Topologies of convergences for discrete-to-continuum limit on Poisson point clouds
- [03219] Spectral Methods for Data Sets of Mixed Dimensions
- [03228] An information geometric and optimal transport framework for Gaussian processes
- [03101] Data analysis and optimal transport: some statistical tools
- [02871] Multispecies Optimal Transport and its Linearization
- [03196] Semi-supervised learning with the p-Laplacian
- [03217] The passive symmetries of machine learning
- [03186] Graphons in Machine Learning
- [03178] Graphon Analysis of Graph Neural Networks
- [03202] Graph Neural Networks on Large Random Graphs: Convergence, Stability, Universality

**[00027] Recent trends on crowd management**

- [05480] Crowd Management Platform as a Service
- [05405] 3D Visualization of Crowd Motion
- [05377] Numerical description of pedestrian crowds: are we really particles?
- [05404] Crowd management and visitors' attitudes in natural recreational areas

**[00029] New Trends in Structural and Engineering Optimization**

- [04641] Topology optimization reducing the dynamic instability of squeal noise
- [03974] Structural simulation and optimization to improve the quality of metal additive manufacturing
- [03594] Machine-learning assisted topology optimization with structural gene inheritance
- [03346] Numerical and experimental investigation on process parameters optimization in rapid heat cycle molding
- [01219] Acoustic metamaterials design with non-gradient material-field series-expansion topology optimization
- [04675] Multiscale topology optimization to maximize dissipated energy
- [03135] Multiscale topology optimization of fiber reinforced composite using homogenization design method.

**[00033] Recent Advances on Quantitative Finance**

- [04926] Neural Stopping Boundaries
- [05322] Learning Equilibrium Mean-Variance Strategy
- [05301] On Consistency of Selecting Signatures Using Lasso: A Tale of Ito and Stratonovich
- [02766] Portfolio choice with transaction costs and reinforcement learning
- [05335] Dynamic programming for mean-variance portfolio selection
- [05363] Non-Concave Utility Maximization with Transaction Costs
- [05320] Optimal stopping without time consistency
- [03404] Optimal dividend payout with non-decreasing constraint
- [05500] Extended mean-field control problems with multi-dimensional singular controls
- [05172] Lightning Network Economics: Channels and Topology
- [05309] Non-monotone linear-quadratic mean field games with a major player
- [05501] Large ranking games with diffusion control

**[00036] Different perspectives in non-linear and non-local PDEs**

- [04031] Quantified overdamped limit for Vlasov-Fokker-Planck equations with singular interaction forces
- [04055] A Degenerate Cross-Diffusion System as the Inviscid Limit of a Nonlocal Tissue Growth Model
- [03802] Nonlocal particle approximations of the porous medium equation
- [05056] A convergent discretization of the porous medium equation with fractional pressure
- [05097] Uniform spectral gap in nonlocal-to-local approximations of diffusion
- [03996] Concentration phenomena arising in Aggregation Fast-Diffusion equations
- [05394] Sharp uniform-in-time propagation of chaos on the torus
- [04109] Limiting gradient flow structure of deep linear neural networks
- [04224] Deterministic Particle Approximation for aggregation-diffusion equations: entropy solutions, gradient flows, graph.
- [03893] Non-local PDEs on graphs

**[00037] Recent advances in modelling and simulation of interfacial flows**

- [02292] Interfacial flows and their modelling and control
- [05417] New perspectives on continuous film flow over non-planar substrate: a family affair
- [02788] Nonlinear dynamics of unstably stratified two-layer shear flow in a horizontal channel
- [04110] Neural network methods for solving interface problems
- [05355] On the transition to dripping of an inverted liquid film
- [03447] Influence of an elastic sheet on impact on a liquid surface

- [03420] Spin Coating on a Non-Axisymmetric Curved Substrate
- [05432] Evaporation and the coffee-ring effect for non-circular droplets
- [00038] Frontiers of gradient flows: well-posedness, asymptotics, singular limits**
  - [05191] Existence for a class of fourth-order quasilinear parabolic systems
  - [03572] Evolutionary limit of gradient flows in heterogeneous Wasserstein space
  - [04719] The fourth-order total variation flow in  $\mathbb{R}^n$
  - [05426] Global existence for the p-Sobolev flow
  - [02587] Weak solutions to gradient flows in metric measure spaces
  - [04233] Duality methods for gradient flows of linear growth functionals
  - [04556] Convergence of Sobolev gradient trajectories to elastica
  - [05251] Recent advances in Sobolev gradient flows of plane curves
- [00047] Combining Machine Learning and Stochastic Methods for Modeling and Forecasting Complex Systems**
  - [03378] Generative modelling through diffusion maps
  - [04604] Tracer Prediction in Simplified Stochastic Geophysical Models through Kalman Filters and Related Methods
  - [05043] Machine Learning for Stochastic Parametrisation
  - [03280] Explainable AI to Detect, Predict and Discover Climate Variability and Change
  - [05245] semi-supervised active learning on graphs
  - [04307] Integrating the spectral analyses of neural networks and nonlinear physics for explainability, generalizability, and stability
  - [03737] Shock trace prediction by reduced models for a viscous stochastic Burgers equation
  - [01386] A Multi-Fidelity Ensemble Kalman Filter with Adaptive Reduced-Order Models
  - [05228] Embedding classical dynamics in a quantum computer
  - [05225] Machine learning correction operators for capturing extremes in coarse scale climate models
  - [04015] A Framework for Machine Learning of Model Error in Dynamical Systems
  - [05032] Combining physical and machine learning forecasts for Earth system prediction
- [00048] Interfaces between kinetic equations and many-agent social systems. Part I**
  - [03361] Multi Agent System for Inverse Problems
  - [03822] Parameter estimation for macroscopic pedestrian dynamics models using microscopic data
  - [03518] Navigation system based routing strategies in traffic flows on networks
  - [02357] Uncertainty quantification in vehicular traffic models
  - [04654] On a kinetic Elo rating model for players with dynamical strength
  - [04235] Nonlocal approximation of nonlinear diffusion equations and cross-diffusion systems
  - [04374] Kinetic models for multi-agent systems with multiple microscopic states
  - [03362] Modelling coevolutionary dynamics in heterogeneous SI epidemiological systems across scales
  - [05559] The Collisional Particle-In-Cell Method for the Vlasov-Maxwell-Landau System
- [00049] Interfaces between kinetic equations and many-agent social systems. Part II**
  - [04948] Weak couplings of Lohe type aggregation models
  - [03897] Quantified overdamped limit for Kinetic Vlasov-Fokker-Planck equations
  - [04724] Phase-coupled models for synchronization with nonlocal temporal interactions
  - [04208] Rigorous derivation of the Euler-Alignment model with singular communication weights from a kinetic Fokker-Planck-Alignment model
  - [04945] Sticky-particle Cucker-Smale dynamics and the entropic selection principle for the Euler-alignment system
  - [04190] Structure-preserving particle method for the Vlasov-Landau-Maxwell system
  - [03372] On solutions to the kinetic Cucker-Smale model with singular communication weights
  - [03940] Interaction energy minimizers on bounded domains
  - [03933] Analytical approaches to the problem of emergence arising in systems of collective behavior
- [00052] Efficient numerical methods for high-dimensional PDEs**
  - [04856] Sparse grid techniques for particle-in-cell simulation of kinetic plasmas
  - [03639] Nonlinear model reduction with adaptive bases and adaptive sampling
  - [04871] Quantum Algorithms for Accelerating the Solution of Partial Differential Equations
  - [03854] A Hybrid AMR Low-Rank Tensor Approach for Solving the Boltzmann Equation
  - [04128] Designing High-Dimensional Closed-Loop Optimal Control Using Deep Neural Networks
  - [04563] An Inverse Problem in Mean Field Games from Partial Boundary Measurement
  - [04470] Automatic partitioning for Boolean CME Low-Rank integrator
- [00057] Many-agent systems and mean-field models for socio-economic and life sciences dynamics**
  - [04044] Data-driven kinetic model for opinion dynamics and contacts
  - [02360] Asymptotic-preserving neural networks for kinetic equations in socio-epidemics
  - [04507] Many-agent systems and mean-field models for semi-supervised learning
  - [03820] Trends to equilibrium for nonlocal Fokker-Planck equations with discontinuous drift
  - [04768] Kinetic modelling of swarming dynamics with transient leadership
  - [02465] Kernel learning method for multiagent systems and its mean-field limit
  - [03937] Bounded-confidence models of opinion dynamics on networks
  - [03493] Mean-field models for many agent systems with co-evolving network structure
- [00059] Numerical solutions for differential equations: Probabilistic approaches and statistical perspectives**
  - [00066] Probabilistic Numerical Methods
  - [04930] Prior models for enforcing boundary constraints in state-space probabilistic PDE solvers

- [04408] GParareal: Towards a time-parallel probabilistic ODE solver
- [00148] Theoretical Guarantees for the Statistical Finite Element Method
- [00714] Approximating the solutions of delay differential equations via the randomized Euler method
- [00186] Posterior error estimates for statistical finite element methods with Sobolev priors
- [04863] The Bayesian approach to inverse Robin problems
- [02954] Statistical finite elements for misspecified models
- [00060] Mathematical approaches to collective phenomena**
  - [04763] Multi-fidelity method for a class of kinetic equations with uncertainties
  - [04788] Brownian HydroDynamics for Confined Electrolyte Solutions
  - [04809] Delay Models of Collective Behavior with Biological and Industrial Applications
  - [04973] Model Cascades for Dilute Gases Based on Moment Equations
- [00061] Reaction-Diffusion models in Ecology and Evolution**
  - [00123] Propagation direction of the traveling wave in the Lotka-Volterra competition-diffusion system
  - [00124] Principal eigenvalue problem with large advection in 2 dimensional case
  - [00099] Some game theoretical models in population dynamics
  - [00125] Free boundary problem for the curve shortening flow with driving force in undulating cylindrical domains
  - [00120] Front Propagation in the Shadow Wave-Pinning Model
  - [00109] Propagation speeds in a shifting environment
  - [00067] Lotka-Volterra competition-diffusion system: the critical competition case
  - [00080] Coexistence of strains in some reaction-diffusion systems for infectious disease
- [00062] Analysis and computation of vortical flows**
  - [00106] Logarithmic vortex spirals
  - [00069] Dynamics of elliptical vortices
  - [00121] The N-vortex problem in doubly-periodic domains with background vorticity
  - [00127] Swimming of a Fish-like Body by using a Vortex Shedding Model
  - [00075] Motion of three geostrophic vortices
  - [00126] Self-similar vortical flows
  - [00150] Near-singular integrals in 3D interfacial Stokes and potential flows
  - [00147] The FARSIGHT Vlasov-Poisson code
- [00063] Recent Advances on Nonlocal Interaction Models**
  - [04295] Patterns in block copolymers
  - [00152] Patterns in tri-block copolymers: droplets, double-bubbles and core-shells.
  - [00113] Ground states for aggregation-diffusion models on Cartan-Hadamard manifolds
  - [00101] Well-posedness and asymptotic behaviour of an interaction model on Riemannian manifolds
  - [00131] Mean field games with aggregating interaction potentials of nonlocal type
  - [00105] Deterministic particle approximation for a nonlocal interaction equation with repulsive singular potential
  - [00155] Nonlocal deterministic and stochastic models for collective movement in biology
  - [00117] Zero-Inertia Limit: from Particle Swarm Optimization to Consensus-Based Optimization
  - [00093] Many-spike limits of reaction-diffusion systems of PDEs
  - [00157] Pattern formation in particle systems: spherical shells to regular simplices
  - [05071] Some remarks on minimization of nonlocal attracting repulsing energies
  - [00145] On a Becker-Döring model for prions and an associated nonlocal problem.
  - [04453] Shape Optimization for nonlocal anisotropic energies
- [00065] Recent Advances on Stochastic Hamiltonian Dynamical Systems**
  - [04102] The Hamilton-Jacobi Theory for Stochastic Hamiltonian Systems on Jacobi Manifold
  - [02876] Homogenization of Dissipative Hamiltonian Systems under L'evy Fluctuations
  - [02877] The stochastic flocking model with far-field degenerate communication
  - [04106] The Most Likely Transition Path for a Class of Distribution-Dependent Stochastic Systems
  - [00862] A parameterization method for quasi-periodic systems with noise
  - [04265] Parametric Resonance for Enhancing the Rate of Metastable Transition
  - [04127] An end-to-end deep learning approach for extracting stochastic dynamical systems with  $\alpha$ -stable Lévy noise
  - [04130] Schrodinger Meets Onsager
  - [00806] Recent progress in spatial isosceles three body problem
- [00068] Models for collective behavior and emergent phenomena**
  - [03562] Emergence of Biological Transportation Networks as a Self-Regulated Process
  - [03929] Bifurcations in collective dynamics: ordered and disordered behaviour
  - [04259] A new approach to upscaling of KTEs modelling cell migration
  - [04922] Asymptotic limits of transient patterns in a continuous-space interacting particle system.
  - [04504] Model Reduction and Coarse-Graining of Complex Systems
  - [05047] Splitting methods for optimal control
  - [05107] Nonlocal Cross-interaction Systems on Graphs: Energy Landscape and Dynamics
- [00072] Evolution equations in materials science: Multiscale modeling, analysis, and simulation**
  - [04859] Diffusion in the presence of microstructures: Does vesicle micro-dynamics enhance the signalling among plants macro-transport?
  - [04217] Morphology formation in ternary mixtures: A continuum model

[05044] Homogenisation of an advection-reaction-diffusion process in a porous medium with coupled evolving microstructure  
 [04239] Partial differential equations for moisture transport in porous materials

[04230] A two-scale model describing swelling phenomenon in porous materials  
 [04483] Improved corrector regularity in homogenization with non-smooth coefficients  
 [03965] Solvability of a dynamical model for the elastic curves  
 [04592] Numerical simulations and analysis for mathematical modeling of adsorption phenomena

[04388] Decay estimates for a unit cell model of composite materials  
 [04211] Effective hydromechanic models for fibre-reinforced hydrogels  
 [04680] An elastoplastic model with a time-dependent threshold function

#### **[00082] Development in fractional diffusion equations: models and methods**

[00162] Solution of a fractional Stefan problem using a Landau transformation  
 [00166] Fractional diffusion as an intermediate asymptotic regime  
 [02596] Dissipativity of the energy functional in time-fractional gradient flows  
 [00119] Weak and entropy solutions of time-fractional porous medium type equations  
 [00167] On different formulations for time-fractional Stefan problems  
 [00163] Numerical methods for nonlocal and nonlinear parabolic equations with applications in hydrology and climatology  
 [00160] Regularity of weak solutions to parabolic-type problems with distributed order time-fractional derivative  
 [04911] Uniqueness for inverse source problems for time-fractional diffusion-wave equations  
 [02617] Fractional diffusion equation with psi-Hilfer derivative  
 [02623] On the  $\psi$ -Hilfer time-fractional telegraph equation in higher dimensions  
 [02767] The fundamental solution to the space fractional diffusion equation

#### **[00084] Asymptotic approaches to multi-scale PDEs in mathematical physics**

[04992] Relative entropy and application to asymptotic limits for bipolar Euler-Poisson systems.  
 [04461] From compressible euler equation to porous media  
 [03337] On the asymptotic dynamics of point vortices for the lake equations  
 [03190] Strong Convergence of Vorticity in the Viscosity Limit  
 [05460] Local smooth solvability for the Relativistic Vlasov-Maxwell system.  
 [04487] Incompressible limit for tumor growth models with convective effects  
 [03628] Construction of weak solutions to Compressible Navier-Stokes equations

#### **[00085] Singular Problems in Mechanics**

[00222] Recent progress on the irreversible fracture phase field model  
 [00267] Fractional Korn inequalities in bounded domains  
 [00266] On Phase Field Approach for Crack Propagation due to Water Pressure in Porous Medium  
 [00171] Asymptotic series solution of variational Stokes problems in planar domain with crack-like singularity  
 [00288] Evolution equations with complete irreversibility  
 [00285]  $H^2$ -regularity up to boundary for a Bingham fluid model  
 [00279] On a generalization Kelvin-Voigt model with pressure-dependent moduli  
 [00287] A reconstruction problem in nanoscale processing by transverse dynamic force microscopy  
 [00203] On Kirchhoff-Love plates with thin elastic junction  
 [00235] Optimal Location Problem for Heterogeneous Bodies with Separate and Joined Rigid Inclusions  
 [00210] Multiscale analysis of stationary thermoelastic vibrations of a composite material  
 [00207] An impulsive pseudoparabolic equation with an infinitesimal transition layer

#### **[00086] Recent advances in the theory of rogue waves: stability and universality of wave pattern formation**

[05527] Universal rogue wave patterns and their connections with special polynomials  
 [05532] Determinant formula for Rogue waves and the binomial theorem  
 [05549] Two-dimensional rogue waves generated by resonance collision  
 [04902] Rogue waves of infinite order and their properties, Part 1  
 [04895] Rogue waves of infinite order and their properties, Part 2  
 [05529] Universality and rogue waves in semi-classical sine-Gordon equation  
 [05518] Large order breathers of the nonlinear Schodinger equation  
 [04536] On stability of KdV solitons  
 [05530] Rogue waves in the massive Thirring model  
 [03606] Resonant breather and rogue wave solutions to a coupled Sasa-Satsuma equation  
 [03607] Resonant breather and rogue wave solutions to a coupled Sasa-Satsuma equation

#### **[00087] Intersection of Machine Learning, Dynamical Systems and Control**

[02826] Solving Parametric PDEs by Deep Learning  
 [02805] Training Deep ResNet with Batch Normalization as a First-order Mean Field Type Problem  
 [02933] Dynamics-Quantified Implicit Biases of Large Learning Rates  
 [04799] An optimal control perspective on diffusion-based generative modeling leading to robust numerical methods  
 [04826] Learning high-dimensional feedback laws for collective dynamics control  
 [05378] Sparse Kernel Flows for Learning 132 Chaotic Dynamical Systems from Data  
 [05395] Distributed Control of Partial Differential Equations Using Convolutional Reinforcement Learning

#### **[00088] Machine learning in infinite dimensions**

[02760] Approximation by structured deep neural networks  
 [03794] Learning High-Dimensional Banach-Valued Functions from Limited Data with Deep Neural Networks

- [04519] Kernel methods for learning operators between infinite dimensional Banach spaces
- [03223] A duality framework for generalization analysis of random feature models and two-layer neural networks
- [03216] Reliable extrapolation of deep neural operators informed by physics or sparse observations
- [04824] Analysis of Neural Networks : Blessings of Width, Curses of Depth
- [02466] Mirror Descent with Relative Smoothness in Measure Spaces, with application to Sinkhorn and EM
- [05291] Covariance-Modulated Optimal Transport Geometry
- [04018] Learning PDE operators with neural networks
- [04864] Learning solution operators for PDEs with uncertainty
- [04774] Unsupervised Learning of the Total Variation Flow
- [03051] On solving/learning nonlinear PDEs with GPs

**[00090] Recent advances in the theory of rogue waves: one- and multi-component models in 1+1 and 2+1 dimensions**

- [03779] Maximal Amplitudes of N-Phase Solutions of a Modified NLS Equation
- [05214] The effects of damping on rogue wave formation and permanent downshifting
- [04450] Rogue-wave formation scenarios for focusing NLS with parabolic initial data
- [04494] Stability of plane waves for the Yajima-Oikawa-Newell equation
- [04830] Rogue waves in 1+1 and in 2+1 dimensions
- [04499] Finite-gap approach to the Davey-Stewartson-2 rogue waves
- [04876] Non-commutative soliton equations: some solutions of matrix mKdV equation
- [05198] Spectral approaches to wave instability

**[00107] Randomized numerical linear algebra**

- [03344] Randomized low-rank approximation: Where we've been and where we're going
- [04049] Efficient Bounds for Canonical Angles in Randomized Subspace Approximations
- [03767] Randomized Nyström approximation for symmetric indefinite matrices
- [04567] The Cluster and the Gap in Randomized Subspace Iteration
- [04958] RandNLA for Faster Convex Optimization
- [03373] Sketched Gaussian Model Linear Discriminant Analysis via the Randomized Kaczmarz Method
- [03665] Moment Estimation of Nonparametric Mixtures Through Implicit Tensor Decomposition
- [04802] Are sketch-and-precondition least squares solvers numerically stable?
- [04913] RandBLAS and RandLAPACK - Toward Standard Libraries for RandNLA
- [04810] Error Estimation in Randomized Algorithms for Rank-Revealing Factorizations
- [04484] Krylov-aware stochastic trace estimation
- [04463] How and why to "uncompute" the randomized SVD

**[00108] Recent Advances on Kinetic and Related Equations**

- [01451] Boundary singularity of a mono-speed Lorentz model for molecules with the infinite-range potential
- [01849] On the Existence and Regularity for the Stationary Linearized Boltzmann Equation in a Small Domain
- [05464] Regularity estimates for the non-cutoff soft potential Boltzmann equation with typical rough and slowly decaying data
- [00646] Vanishing angular singularity limit to the hard-sphere Boltzmann equation
- [04112] On BGK-type models with velocity-dependent collision frequency
- [02844] Green's function for solving IBVP of evolutionary PDEs
- [00644] H<sup>1</sup>OLDER REGULARITY OF THE BOLTZMANN EQUATION PAST AN OBSTACLE
- [03811] Solution to the Boltzmann equation without cutoff in  $(L^1 \cap L^p)_k$
- [01835] Mixture estimate in fractional sense
- [03301] Dynamical behaviors in stochastic kinetic flocking models
- [04712] Kinetic study of a gas undergoing resonant collisions

**[00110] Computation on Supersingular and Superspecial Curves and its Applications**

- [04024] Decomposed Richelot isogenies of Jacobian varieties of hyperelliptic curves and generalized Howe curves
- [04668] Some explicit arithmetics on curves of genus three and their applications
- [05345] Construction of superspecial curves of higher genera with extra automorphisms
- [04048] Several examples of curves whose superspeciality imply maximality or minimality

**[00114] Computational Biology**

- [05357] Different mathematical models for membrane electroporation: from equivalent circuit to phase-field models
- [02031] Modeling and characterizing vaccine-elicited antibody responses
- [03370] Mathematical analysis of bone metabolism markers in immobilization mice
- [02284] Predicting clinical outcomes of acute liver failure
- [03648] Mathematical investigation into the mechanism of hair follicle morphogenesis
- [03506] Parameter estimation of the compartmental model of systemic circulation describing the Glucose, Insulin and C peptide dynamics
- [02898] Effective nonlocal kernels on Reaction-diffusion networks
- [04349] Mathematical model of mTORC1 pathway sensing intracellular amino-acids and glucose
- [05379] Mathematical modeling of cancer immune escape
- [02179] Computational modelling of cancer invasion using organotypic invasion assay data
- [05467] The prognostic value of immune infiltration patterns on the outcome of chemotherapy in breast cancer

**[00118] On mathematical modeling and simulation of droplets**

- [03374] Plug formation in models of falling viscous films inside tubes
- [03547] Dipole-type solutions to the thin-film equation

- [02422] Thermally-driven coalescence in thin liquid film flowing down a fiber
- [01886] Hybrid Asymptotic-Numerical Methods for Two-Phase Flow With Soluble Surfactant
- [01260] A phase field model for a drop suspended in viscous liquids under the influence of electric fields
- [05478] Phase-field modeling of colloid-polymer mixtures in microgravity
- [02884] Capillary rebound of droplets impacting onto a liquid bath
- [01510] Motion of Liquid Droplets in Gas Channels
- [02886] On the immersed boundary method in simulating liquid-gas interfaces

**[00134] Evolution Equations for Interacting Species: Applications and Analysis**

- [05128] Evolution Equations for Interacting Species: Applications and Analysis
- [05084] A Keller-Segel type approximation to a cell population dynamics model
- [04550] Convergence of position-based dynamics for first-order particle systems with volume exclusion
- [04803] Graph-to-local limit for the nonlocal interaction equation
- [05193] A model for territorial dynamics: from particle to continuum
- [04662] A variational approach for an existence result for a cross-diffusion model
- [04745] A degenerate cross-diffusion system as the inviscid limit of a nonlocal tissue growth model
- [04637] Proposing a Finite Volume Method for a Kinetic Model for Interacting Species
- [05038] Mean-field convergence in  $L^2$ -norm for a diffusion model with aggregation
- [04613] Macroscopic limits of kinetic equations for the switch in cell migration via binary interactions
- [04647] Towards a new mathematical model of the visual cycle
- [04418] Structured Model for the Size-spectrum Evolution in Aquatic Ecosystems

**[00135] Nonlinear PDEs and related diffusion phenomena**

- [03392] Boundary Regularity of Local and Nonlocal Equations
- [04308] Well-posedness with large data for a weighted porous medium equation
- [04047] Results on the Stokes eigenvalue problem under Navier boundary conditions
- [03585] Weighted Trudinger-Moser inequalities in the subcritical Sobolev spaces
- [03273] First order fully nonlinear nonlocal evolution equations
- [02461] The generalized porous medium equation on graphs: Existence and uniqueness of solutions with  $l^1$  data
- [03236] Global regularity estimates for the Poisson equation on complete manifolds
- [03203] Radial solutions to a semilinear equation on Riemannian models
- [03548] Quasi self-similarity and its application to the global in time solvability of a superlinear heat equation
- [03604] Stochastically perturbed log diffusion equations
- [03225] Spreading and extinction of solutions to the logarithmic diffusion with a logistic reaction
- [03474] Characterization of F-concavity preserved by the Dirichlet heat flow

**[00137] Mathematical Aspects of Multiscale Phenomena in Materials and Complex Fluids**

- [00142] New perspectives on modeling and analysis of grain growth in polycrystals
- [00183] Entropy dissipation methods for Nonlinear inhomogeneous Fokker-Planck models
- [00198] Structure-preserving variational discretizations to generalized gradient flows
- [00248] Towards upscaling and simulation of coupled [THM] systems with applications to permafrost modeling
- [00202] Diffuse-interface approach to competition between viscous flow and diffusion in pinch-off dynamics
- [00195] Multiscale analysis of nonlinear material models with carrier kinetics
- [00209] Energetic-variational particle-based method for Fokker-Planck Models.
- [00214] Phase transitions in near-liquid solids
- [00243] A finer singular limit of the Kobayashi-Warren-Carter type functional and its gradient flow
- [00249] Variational modeling of fluid in poroelastic medium
- [00226] Phase field model for volume-preserving mean curvature flow
- [00257] A unified continuum model for grain boundary dynamics incorporating microscopic structure

**[00140] Interacting particle systems: modeling, learning and applications**

- [03778] The mean-field limit of non-exchangeable integrate and fire systems
- [03624] Weak Form Equation Learning for Interacting Particle System Models of Collective Motion
- [03774] Mean-field nonparametric estimation of interacting particle systems
- [04754] Game-based learning of interaction rules for rational agents
- [04464] Data-driven discovery of interacting particle systems with Gaussian Processes
- [03149] The mean field limit of random batch interacting particle systems
- [04827] Neural parameter calibration for large-scale multi-agent systems
- [05244] Non-local regularization of Semilinear PDE for Probability Density Stabilization

**[00143] Recent advances in stochastic optimal control and contract theory**

- [00182] Mean field optimal stopping and applications in contract theory
- [00242] A stochastic target approach to Stackelberg games and moral hazard with constraints
- [05385] Asset Bubble Riding with Price-Dependent Entry: a Mean Field Game of Controls with Common Noise
- [05410] Bubble Riding with Price-Dependent Entry: Mean Field Games of Controls with Common Noise

**[00151] Recent trends in SHM: damage modeling and optimal experimental design from a mechanical and mathematical point of view**

- [00271] Optimization aspects of experimental design approaches for sensor placement
- [00272] Fracture propagation by using shape optimization techniques on Riemannian spaces
- [00246] Numerical modeling of crack propagation in concrete by means of cohesive zone modeling and a novel phase-field fracture approach

- [00231] Sequential subspace optimization for recovering stored-energy functions in hyperelastic materials
- [00230] A low power autonomous SHM node for aerospace applications
- [00270] Damage parameter estimation in composite materials using data assimilation with reduced order models
- [00256] Coefficient Control for Variational Inequalities
- [00269] Optimal sparse sensor location for structural health monitoring

**[00153] Recent Advances on Inverse Analysis**

- [01421] Tidal current estimation based on the extended Kalman filter FEM
- [01427] Optimal shape design of auxetic structures with periodicity
- [01428] Density-based topology optimization using a modified optimality criteria method
- [03034] Shape Design Problems Considering Fluid-Structure-Interactive Fields

**[00154] Homogenization of PDEs in domains with oscillating boundaries or interfaces**

- [00392] Asymptotic analysis of a parabolic problem with a rough fast oscillating interface
- [00417] A decomposition result for thin domains with rough boundary
- [00412] Derivation of coupled Stokes-Plate-Equations for fluid flow through thin porous elastic layers
- [00416] Homogenization of a two-component domain with an oscillating thick interface
- [00402] Heat conduction in composite media involving imperfect contact conditions
- [00399] Homogenization by unfolding of a Bingham fluid in a thin domain with rough boundary
- [00401] Homogenization of Stokes system with Neumann condition on highly oscillating boundary
- [00407] Fluids with a non-slip condition on a non-periodic oscillating boundary

**[00164] Recent Advances in Direct and Inverse Problems in Mathematical Materials Science**

- [00473] Bloch Waves in High Contrast Electromagnetic Crystals
- [00483] An axisymmetric problem for a nano-sized material surface on a boundary of an elastic semi-space
- [00569] Clusters of Bloch waves in three-dimensional periodic media
- [00588] Modeling sea ice as a multiscale composite material
- [00596] Forward and inverse homogenization for quasiperiodic composites
- [00609] Studying Stefan problems with internal heat generation using sharp interface models
- [00623] Capturing Quasistatic Fracture Evolution with Nonlocal Models
- [00631] The Lippmann-Schwinger-Lanczos algorithm for inverse scattering problems
- [00647] Uncertainty quantification for stochastic models of damage mechanics
- [00649] On the governing equations of poro-piezoelectric composite materials
- [01237] Homogenization of a suspension of viscous fluid with magnetic particles
- [05177] Energy-efficient flocking of particle systems

**[00168] Applications of evolutionary algorithms in differential equation models**

- [03121] Spherical search with multi-operator differential evolution for constrained optimization problems
- [02925] Minimizing infections and intervention cost: multi-objective approach with user-friendly dashboard
- [02755] Comparative Study of Heuristic Algorithms for Electrical Impedance Tomography
- [03163] Bi-objective optimization considering bed capacity and timing of interventions

**[00170] Integrable systems, orthogonal polynomials and asymptotics**

- [05493] Welcome and Introduction
- [02937] Lagrangian multiform structure of discrete and semi-discrete KP typeequations
- [03500] Charge-conserving solutions to the constant Yang-Baxter equations
- [03983] Stokes' phenomenon, discretization, and discrete integrability
- [04872] On q-Painlevé VI and the geometry of affine Segre surfaces
- [04990] Deformed orthogonal functions and integrable lattices
- [05269] Borel analysis for the first difference q-Painlevé equation
- [05326] Non-linear Stokes phenomenon for Painleve transcedents and topological recursion
- [05494] Orthogonal polynomials on elliptic curves and Painlevé VI equation.
- [05496] Asymptotic prediction of tau-function zeros of Painlevé equations
- [05564] Riemann-Hilbert problem on the q-Painleve equations
- [05591] A 3x3 Lax form for the q-P(E\_6^(1))

**[00172] On application of principle curvature distribution in local differential geometry**

- [04166] Fullerene and discrete principal curvature
- [03759] Interplay between topology-induced geometry and the electronic properties of nanocarbon materials
- [04350] On discrete constant principal curvature surfaces
- [04368] Surface parametrization for manufacturing by principal curvature integral

**[00176] Hyperbolic PDEs modelling non-Newtonian fluid flows**

- [00332] Well-posedness and asymptotic behavior for hyperbolized compressible Navier-Stokes equations
- [00503] Structure preserving finite element schemes for a non-Newtonian flow
- [00918] Temporal discretisation of non-Newtonian fluid flows
- [04850] New symmetric-hyperbolic PDEs for viscoelastic fluid flows

**[00178] Theoretical and Computational Progress on PDE-based Inverse Problems with Applications**

- [00556] Deterministic-Statistical Approach for Inverse Problems with Partial Data
- [00553] Quantitative PAT with simplified PN approximation
- [02856] Adaptive Mesh-free Approach for Gravity Inversion
- [00358] A neural network method for inverse source problem with limited-aperture data
- [00236] On plasmon modes in multi-layer structures

- [00405] Uniqueness and non-uniqueness for inverse source problems of elliptic equations
- [00361] Mathematical analysis of microscale hydrodynamic cloaking and shielding using electro-osmosis
- [00920] Regularizing Effect of Damping Mechanisms in Inverse Problems of Evolution Equations
- [00359] A NOVEL QUANTITATIVE INVERSE SCATTERING SCHEME USING INTERIOR RESONANT MODES
- [00333] Simultaneous recovery of a scattering cavity and its internal sources
- [00259] The anisotropic Calderón problem at large fixed frequency on manifolds with invertible ray transform
- [00245] Minnaert resonances for bubbles in soft elastic materials
- [00179] Advances in forward and inverse problems of wave equations**
  - [00347] Accurate evaluation of Helmholtz layer potentials using Quadrature by two expansions
  - [00411] On the Robustness of Inverse Scattering for Penetrable, Homogeneous Objects
  - [00490] A Neural Network Warm-Start Approach for the Inverse Acoustic Obstacle Scattering Problem
  - [04073] Optimal Transportation for Electrical Impedance Tomography
  - [03446] A high-accuracy boundary integral equation method for wave scattering by 3D analytic surfaces
  - [03520] Fast algorithms for multiple elastic obstacles scattering and inverse scattering
  - [05069] Exploring inverse obstacle scattering with an impedance model
  - [03858] Hybrid methods for the application of singular integral operators
  - [04029] Obstacles and interfaces composite scattering in a multilayered medium
  - [04887] Lippmann-Schwinger integral equation for fiber optics analysis
  - [05178] Single-excitation quantum optics: analysis and algorithms
  - [05639] Poisson Solver for Complicated Geometries in R3 Using Function Extension
- [00184] Recent advances in data-driven methods for inverse problems**
  - [05418] Machine learned regularization for inverse problems - the dos and don'ts
  - [04644] Data-driven Regularization based on Diagonal Frame Decomposition
  - [03944] Fourier Neural Operators for data-driven regularization
  - [05027] Data-driven regularization theory of invertible ResNets for solving inverse problems
  - [05430] Are neural operators really neural operators?
  - [04722] Plug-and-Play Models for Large-Scale Computational Imaging
  - [02097] Learned proximal operators meets unrolling for limited angle tomography
  - [04626] Plug-and-Play sampling for inverse problems in imaging
  - [03828] Recent advance of diffusion models in inverse problems
  - [04409] Conditional Image Generation with Score Based Models
  - [01555] Data-Driven Convex Optimization via Mirror Descent
  - [03784] Multi-Modal Hypergraph Diffusion Network with Dual Prior for Alzheimer Classification
- [00185] AAA rational approximation: extensions and applications**
  - [02196] Review of AAA approximation
  - [05528] pAAA for multivariate functions and AAA-LQO for systems with quadratic outputs
  - [02708] Rational approximation for noisy data
  - [03138] SO-AAA: learning systems with second-order dynamics
  - [02698] Linearization of dynamical systems using the AAA algorithm
  - [02371] Time-domain model reduction in the Loewner framework
  - [05435] AAA and numerical conformal mapping
  - [05536] AAA rational approximation on a continuum
- [00187] Analysis and geometry of inextensible materials**
  - [02002] Modeling and Simulation of Thin Sheet Folding
  - [02066] Periodic partitions with minimal perimeter
  - [02439] Inextensible elastic curves and subriemannian manifolds
  - [02016] Gradient flows of inextensible networks
- [00193] Adversarial robustness at the interface of analysis, geometry and statistics**
  - [00265] Distributionally Robust Gaussian Process Regression and Bayesian Inverse Problems
  - [01932] Adversarial distributional robustness from Wasserstein ascent-descent particle dynamics
  - [00273] Optimal Algorithms for Stochastic Nested Composition Optimization with Applications to Robust Training
  - [00274] Convergence of GDA for mean field two-player zero-sum games
  - [00292] Gamma convergence of a nonlocal perimeter from adversarial machine learning
  - [00313] Provable Adversarial Robustness via Optimal Transport
  - [00277] Adversarial learning and the Wasserstein barycenter problem
  - [00299] Optimal Adversarial Classification: geometry, regularity, and topology
  - [00330] Adversarial flows
  - [02000] Distributionally Robust Linear Predictors using the Max-Sliced Wasserstein Metric
  - [00352] Minimax results for Surrogate risks in Adversarial Learning
  - [00349] Robust second-order estimation algorithms
- [00194] Recent Progress of Computational Electromagnetics**
  - [03979] Application of POD to solve non linear magnetoquasistatic FE problems
  - [04030] BDD-DIAG Preconditioner of the Interface Problem for Magnetostatic Domain Decomposition Analysis
  - [04666] Reduced Order Modeling of a Cage Induction Motor with Skewed Rotor Slots
  - [05040] Introducing extended finite element approaches in eddy currents analysis
- [00196] Recent development of mathematical geophysics**

- [01262] Global solutions for rotating MHD equations in the critical space
- [02684] Multi-scale interaction of tropical weather in a simplified three-dimensional model
- [00606] Eigenvalue Problem for Perturbation Operator of Two-jet Kolmogorov Type Flow
- [00377] On the physics-informed neural networks approximating the primitive equations

**[00201] Data-Driven Methods for Rough PDEs**

- [04969] Operator Learning by Regressing PDEs
- [05235] Neural Operator for Discovering Physical Equations
- [05013] Neural Option Pricing for Rough Bergomi Model
- [05221] One shot learning of stochastic differential equations with kernel methods
- [03744] GMsFEM based multiscale model learning
- [03131] Multilevel Picard Approximation Algorithm for Semi-linear Integro-differential Equations
- [03090] Exponentially Convergent Multiscale Finite Element Method
- [05179] Learning Solutions to Elliptic PDEs with Discontinuous Multiscale Parameters
- [04555] Recent Advances in Rigorous Koopmanism
- [05147] Solving path-dependent PDEs with signature kernels
- [05248] Kernel Methods for Rough PDEs

**[00211] Mathematics of Geometric Deep Learning**

- [01563] Negative sampling for graph neural networks based on determinantal point processes
- [01565] Spherical Framelets with Directionality for Spherical Neural Networks
- [01568] Some Applications of Hyperplane Arrangements in Deep Learning
- [01769] Machine Learning in Banach Spaces: A Black-box or White-box Method?
- [01857] Stable Hyperbolic Neural Networks for Graph Generation and Classification
- [02110] Spectral-Inspired Graph Neural Networks
- [02341] Generalization Capabilities of Graph Neural Networks
- [03411] On the stability of spectral graph filters and beyond
- [03588] Geometric Diffusion Generative model for protein sequence design
- [03727] FoSR: First-order spectral rewiring for addressing oversquashing in GNNs
- [04482] DynG2G: An Efficient Stochastic Graph Embedding Method for Temporal Graphs
- [04999] On oversquashing and expressivity: can GNNs mix variables?
- [05074] Applied harmonic analysis and particle dynamics for designing neural message passing on graphs
- [05109] Geometric Deep Learning from a Topological Viewpoint
- [05231] Ridgelet Transforms of Neural Network on Manifolds and Hilbert Spaces
- [05341] Scattering Message Passing

**[00215] Mathematical Advances in the nonlinear PDEs from physics**

- [04052] Wave propagation and stabilization in the Boussinesq-Burgers system
- [03930] Hypersonic similarity for steady potential flows over a two dimensional wedge
- [05017] Stability theory for the linear symmetric hyperbolic system with general relaxation
- [00454] Stability of Riemann shock wave via the method of a-contraction of shifts
- [03959] Polynomial tail solutions for Boltzmann equation in the whole space
- [02793] Analytic regularization effect for the spatially inhomogeneous Boltzmann equation
- [04010] Dispersive limit of kinetic models for collisional plasma
- [04067] Wave propagation and stabilization in the Boussinesq-Burgers system
- [04667] Vacuum free boundary problems in ideal compressible MHD
- [01253] Well-posedness of some free boundary problems in compressible fluids
- [04043] Long time instability of compressible symmetric shear flows

**[00216] Recent Advances on interfaces dynamics modeling and simulation**

- [01225] Solving elliptic interface problems using neural networks
- [01276] Role of Cohesive Fiber-Fiber Interactions in Fibrin Networks
- [01217] Variational Lagrangian schemes for interface problems
- [01256] Helical organization of DNA-like liquid crystal filaments in cylindrical viral capsids
- [01231] A phase-field model and an energy-law preserving method for vesicles
- [01214] Free boundary problems in cardiovascular diseases
- [05636] Buckling on Erythrocyte Membranes in Narrow Capillary Flows
- [01394] Machine Learning of Self Organization from Observation
- [01249] A phase field model for droplets suspended in electrolyte solution
- [01220] A deterministic particle simulation for micro-macro viscoelastic flows
- [01227] A Bubble Model for the Gating of Kv Channels

**[00217] Integration of modeling and data analysis on molecular, cellular, and population dynamics in the life sciences**

- [01180] Mathematical Models of Plasmid Loss
- [00813] Morphology of organoids using a multicellular phase-field model
- [00720] Mind the gap: The extra-embryonic space is crucial geometric constraints regulating cell arrangement.
- [03207] Test three different models for the Chlamydia developmental cycle with intrinsic noise
- [03206] Network design principle for biological dual functions
- [03385] Density Physics-Informed Neural Network infers an arbitrary density distribution for non-Markovian system
- [02263] Integrating different layers of biological data to enhance prediction
- [03677] Physics of Furrow Ingression in C. elegans Zygote

- [01465] Screening cell-cell communication in spatial transcriptomics via collective optimal transport
- [04188] A Novel Tool for Enhanced Single-cell RNA Sequencing Data Preprocessing and Dimensionality Reduction
- [00602] Adaptive immune discrimination of antigen risks by predictive coding

**[00220] Reaction-Diffusion Systems and Applications in life Sciences**

- [01711] Propagation dynamics of the Fisher-KPP nonlocal diffusion equation with free boundary
- [03297] propagation phenomena of fractional diffusion equations
- [02984] Sharp traveling waves for degenerate equations with time-delay: Fisher-KPP equations and Burgers equations
- [03485] Accelerating propagation in a nonlocal model with periodic time delay
- [01484] Recent Progress on Reaction-Diffusion Systems and Applications in Life Sciences
- [04053] Effect of density-dependent dispersal on the predator-prey system
- [04100] Nonlinear Stefan problem with a certain class of multi-stable nonlinearity
- [01531] Some results on a haptotaxis model of cancer invasion
- [05208] Basic Propagation Number

**[00221] Analysis of Fluid Dynamics and Free Boundary Problems**

- [03643] Transonic flows and free boundary problems in gas dynamics
- [03380] Regularity and asymptotics for porous medium equations in bounded domains
- [03966] Energy concentration and weak stability in fluid dynamics
- [03949] On Ericksen-Leslie system with free boundary
- [00618] L1 maximal regularity and its application to the Navier-Stokes equations
- [03780] Fluid flow on surfaces
- [04880] The Curve Shortening Flow for Immersed Curves
- [03690] On a thermodynamically consistent model for magnetoviscoelastic fluids in 3D
- [04664] On some contact angle problems in fluid dynamics
- [00258] The relativistic Euler equations with a physical vacuum boundary

**[00223] Stochastic optimization and stochastic variational inequalities**

- [02880] Dynamic Stochastic Projection Method for Multistage Stochastic Variational Inequalities
- [02891] A two-stage stochastic variational inequality model
- [02899] Discrete approximation for two-stage stochastic variational inequalities
- [05136] Iteratively sampling scheme for stochastic optimization with variable number sample path

**[00232] Theoretical foundations and algorithmic innovation in operator learning**

- [03323] BelNet: basis enhanced learning, a mesh-free neural operator
- [01354] The curse of dimensionality in operator learning
- [05247] Score-based Diffusion Models in Function Space
- [04771] Deep Learning Theories for Problems with Low-Dimensional Structures
- [04076] Local approximation of operators
- [04141] Neural operator surrogates for Gaussian inputs
- [03497] Derivative-Informed Neural Operators for Scalable and Efficient UQ
- [05169] Deep Operator Network Approximation Rates for Lipschitz Operators
- [02675] Transfer Learning Enhanced Physics-informed DeepONets for Long-time Prediction
- [03360] Generic bounds on the approximation error for physics-informed (and) operator learning
- [03124] Overcoming Fundamental Limitations of Current AI Approaches: From Digital to Analog Hardware

**[00234] Differential Galois Theory and Integrability of Dynamical Systems**

- [05314] The geodesic deviation equation for null geodesics in the Schwarzschild black-hole
- [03161] Non-integrability of a model of two tethered satellites
- [04393] Obstructions to integrability of nearly integrable dynamical systems
- [04873] A Tale of Two Polytopes related to geodesic flows on spheres
- [03566] Local integrability and regularity of autonomous differential systems
- [04369] Singular solitary waves in the KdV equation
- [04649] Korteweg-de Vries traveling waves and Differential Galois Theory
- [03529] Real Liouvillian extensions of partial differential fields

**[00237] Recent progress in multiscale modeling and computational methods in material sciences**

- [05400] Numerical methods for topology optimization and applications
- [05389] Optimal error estimate for the Multiscale Finite Element Method
- [05618] On median filters for motion by mean curvature
- [02920] Structure-preserving methods based on minimizing movement scheme for gradient flows with respect to transport distances
- [05350] Multi-scale modeling and simulations for two-phase flow with moving contact lines
- [04103] Energy stable methods for two-phase phase-field surfactant model
- [01396] Construction and Analysis for the Coupling Method of Atomistic and Higher Order Continuum Models
- [01316] A domain decomposition method for the Poisson-Boltzmann solvation model
- [01430] A Continuum Model for Dislocation Climb Velocity and Numerical Simulations
- [01298] A second-order in time, BGN-based PFEM for solving geometric PDEs

**[00239] Shape and Topology Optimizations**

- [00244] PDEs for topology optimization considering manufacturability
- [00368] Topology optimization of supports for additive manufacturing with accessibility constraints
- [03408] Dehomogenization in stress minimization problems

- [03530] The topological ligament: an approach based on thin tubular inhomogeneities
- [00419] Level set-based topology optimization method with nonlinear diffusion
- [00247] Interfaces and Free Boundaries in Fluid Mechanics and Materials Science**
  - [02095] On the notion of generalized mean curvature flow
  - [03166] Coarsening phenomena in the network flow
  - [03048] Uniqueness and stability of multiphase mean curvature flow beyond a singular time: the case of the shrinking circle
  - [02872] Matrix-valued Allen–Cahn equation and the Keller–Rubinstein–Sternberg problem
  - [03054] Variational methods for time-dependent problems on dynamically changing domains
  - [04468] Sharp-interface limit of models with mechanics and contact lines
  - [03766] Uniform Rectifiability for Minimizers of the Griffith Fracture Energy
- [00253] Modelling and Simulation of Lithium-Ion Batteries**
  - [03631] Asymptotic methods for lithium-ion battery models
  - [05237] Topology Optimization for Li-ion batteries
  - [04263] Homogenisation and Modelling of a Silicon nanowire Li-ion battery anode
  - [02731] A continuum model for lithium plating and dendrite formation in lithium-ion batteries.
  - [04505] Simulation and analysis of space charge layers in a solid electrolyte
  - [03112] Machine Learning of Electrochemistry Battery Models
  - [05150] Parameterisation of reduced-order battery models from non-invasive characterisation
  - [05185] Early prediction of battery remaining useful life using AI and physics
- [00255] Recent developments in fast algorithms for inverse problems and imaging**
  - [03339] Streaming Methods for Inverse Problems
  - [03433] Sequential model correction for nonlinear inverse problems
  - [02062] Plants, robots and dynamic tomography
  - [04602] Deep learning methods for data-driven uncertainty quantification
  - [04412] Exploiting Mixed Precision Arithmetic in Image Reconstruction
  - [03595] Image Quality Assessment for Reconstruction Algorithms
- [00260] Statistics for random dynamics**
  - [03955] Online parametric estimation of stochastic differential equations with discrete observations
  - [03956] Weighted block bootstrap for misspecified ergodic Lévy driven SDE models
  - [04399] Robustifying Gaussian quasi-likelihood inference for random dynamics
  - [04695] Asymptotic expansion of estimator of Hurst parameter of SDE driven by fractional Brownian motion
- [00262] numerical analysis, modeling and applications in phase-field its relevant methods**
  - [05280] Approximating Structurally Unstable Over-determined Systems of PDEs
  - [03012] Energy stability analysis and error estimate of a maximum bound principle preserving scheme for the dynamic Ginzburg–Landau equations under the temporal gauge
  - [04941] Phase-field modelling of three-phase solidification with density variation
  - [02938] Multiscale topology optimization method for lattice materials
  - [04079] New unconditionally stable higher-order consistent splitting schemes for the Navier-Stokes equations
  - [04302] Multi-phase-field modeling of grain growth and multiphase flow in additive manufacturing
  - [04437] An efficient nonsmooth global optimization-based bound-preserving approach for the Cahn-Hilliard equation
  - [05375] Efficient decoupling energy stable approach for coupled type gradient flow systems with anisotropy for alloys
  - [03552] High-order exponential integrators for semilinear parabolic equations with nonsmooth data
  - [04765] Mathematical modeling and numerical approximation of bulk-surface model
  - [02279] Discovery of Governing Equations with Recursive Deep Neural Networks
- [00263] Problems in incompressible fluid flows: Stability, Singularity, and Extreme Behavior**
  - [00695] Enforcing conservation laws in truncated fluid models: the effect on heavy-tailed statistics
  - [00308] Verifying global stability of fluid flows despite transient growth of energy
  - [01836] Invariant solutions representing extreme behaviour in turbulence
  - [03543] Numerical simulation of the convex integration for the dissipative Euler flow
  - [00597] Systematic search for singularities in 3D Euler flows
  - [00371] Mathematical reformulation of the Kolmogorov-Richardson energy cascade in terms of vortex stretching and related topics
  - [03746] Structure and scaling of extremely large velocity gradients in hydrodynamic turbulence.
  - [00303] A model of turbulent flows based on a random Constantin-Lax-Majda-DeGregorio equation
  - [00786] Extending the Gibbon-Fokas-Doering stagnation-point-type ansatz to finite-energy initial conditions: A solution to the Navier-Stokes Millennium Prize Problem?
  - [04968] Singularity detection via regularization: Blow-up criteria for 3D Euler and related equations
  - [02897] Thermalisation in finite-dimensional, inviscid equations of hydrodynamics
  - [00758] How advection delays singularity formation in the Navier-Stokes equations
- [00264] Card-based Protocols and PEZ Protocols**
  - [04248] Physical ZKPs for Logic Puzzles Using a Standard Deck of Cards
  - [05000] Open Problems in Card-Based Cryptography
  - [05052] Recent Progress in Card-Based Cryptography
  - [05471] Introduction to Private PEZ Protocol
- [00268] Neumann—Poincaré Operator, Layer Potential Theory, Plasmonics and Related Topics**
  - [03110] Homogenization and the spectrum of the Neumann Poincaré operator

- [00406] From condensed matter theory to sub-wavelength physics
- [00777] Eigenvalues of zero order pseudodifferential operators and applications to Neumann-Poincare
- [00564] On a uniqueness property of harmonic functions
- [00367] Factorization of Neumann-Poincare operator
- [00452] The quasi-static plasmonic problem for polyhedra
- [00364] Surface localized resonances and applications
- [01244] Spectral structure of the Neumann-Operator on thin domains
- [00730] A unified approach to the field concentration problem
- [00354] Spectral properties of the Neumann-Poincaré operator on rotationally symmetric domains
- [01245] Vector field decomposition and eigenvalues of elastic Neumann-Poincaré operators
- [01265] Essential spectrum of elastic Neumann-Poincaré operators with a corner
- [00662] Fundamental solutions in Colombeau algebra

**[00276] Interplay of Numerical and Analytical Methods in Nonlinear PDEs**

- [05323] Hartree-Fock theory with a self-generated magnetic field
- [02913] Uniform flow in axisymmetric devices through permeability optimization
- [03496] Regularised stochastic Landau-Lifshitz equations and their application in numerical analysis
- [03482] A least squares Hessian/Gradient recovery method for fully nonlinear PDEs in Hamilton-Jacobi-Bellman form
- [01636] Convergent finite element approximation of liquid crystal polymer networks
- [01583] Evolving FEMs with artificial tangential velocities for curvature flows
- [03481] Finite element approximation of implicitly constituted non-Newtonian fluids
- [01330] Error analysis for a local discontinuous Galerkin approximation for systems of p-Navier-Stokes type

**[00278] Nonlocal Modeling, Analysis, and Computation**

- [02501] Coarse-Graining and Nonlocality
- [00366] Wellposedness, regularity, and convergence of nonlocal solutions to classical counterparts
- [00370] Coupling of an atomistic model and peridynamic model using an extended Arlequin framework
- [00445] Local and nonlocal energy-based coupling models
- [01086] Machine-learning based coupling of local and nonlocal models
- [01235] Nonlocal Neural Operators for Learning Complex Physical Systems with Momentum Conservation
- [03023] A Numerical Study of the Peridynamic Differential Operator Discretization of Incompressible Navier-Stokes Problems
- [03546] An efficient peridynamics-based coupling method for composite fracture
- [03632] Nonlocal Boundary Value Problems with Local Boundary Conditions
- [03718] On the optimal control of a linear peridynamic model
- [03800] Nonlocal half-ball vector operators and their applications to nonlocal variational problems
- [05210] CabanaPD: A meshfree GPU-enabled peridynamics code for exascale fracture simulations

**[00280] Canonical Scattering Theory and Application**

- [02735] Diffraction of acoustic waves by multiple independent semi-infinite arrays.
- [05383] Extending the Unified Transform Method for Periodic Scattering Problems
- [01576] A Mathematical Method to Solve Diffraction Problems with Generalised Linear Boundary Conditions
- [03068] Acoustic emission of a vortex ring near a porous edge
- [03187] Spectral computations for defect scattering in disordered topological insulators
- [02368] Analysis of oversampled collocation methods for wave scattering problems
- [03067] Revisiting the frozen-gust assumption for edge scattering using spatially-varying wavepackets
- [03239] Green's function for wave scattering by a semi-infinite flat plate with a serrated edge

**[00283] Recent developments in mathematical imaging and modeling in magnetic particle imaging**

- [03274] The image reconstruction problem in magnetic particle imaging and an application of the deep image prior
- [05253] A hybrid model for image reconstruction in MPI using a FFL
- [04125] MPI using an FFL-scanner: Radon-based image reconstruction for realistic setup assumptions
- [04651] Parameter estimation for modeling of nanoparticle dynamics
- [05030] Implicit neural representations for super-resolution in magnetic particle imaging
- [05026] Reducing displacement artifacts in multi-patch magnetic particle imaging
- [05158] Deconvolution of direct Chebyshev reconstructions in MPI with neural networks
- [04792] A Flexible Approach to Model-Based Reconstruction in Magnetic Particle Imaging
- [04806] Reconstruction of Dynamic Concentrations with Sequential Subspace Optimization
- [04730] Joint motion estimation and image reconstruction for dynamic MPI

**[00286] Low-Reynolds-number swimming: modelling, analysis and applications**

- [03028] Results on Classical Elastohydrodynamics for a Swimming Filament
- [04238] A limiting model for a low Reynolds number swimmer with N passive elastic arms
- [05406] Activation processes of flagellated micro-swimmers
- [02171] Emergent rheotaxis of shape-changing swimmers in Poiseuille flow
- [03303] Nonlinear dynamics, bifurcations and stability transitions in motion of periodically-actuated micro-swimmers
- [05278] Low-Reynolds-number swimming via reinforcement learning
- [03505] Controllability of microswimming systems with and without drift
- [03844] Recent trends in micro-swimming

**[00289] Nonconvex nonlinear programming: Theory and algorithms**

- [02633] A Stochastic Conjugate Gradient Algorithm with Variance Reduction

- [01352] Golden ratio Bregman proximal gradient algorithm for nonconvex optimization problems
- [02076] On the quadratic termination property of the gradient method
- [03083] A novel augmented Lagrangian and its application in linear programming
- [01520] Sensitivity analysis for value functions with application to bilevel programs
- [03119] Extrapolated Bregman proximal difference-of-convex(DC) algorithm for structured DC optimization problems
- [03077] Relaxed constant positive linear dependence constraint qualification for disjunctive programs
- [03103] An Oracle Gradient Regularized Newton Method for Quadratic Measurements Regression

**[00294] Machine Learning and Differential Equations**

- [01809] Certified machine learning: Rigorous a posteriori error bounds for physics-informed neural networks
- [04004] Control of kinetic collective dynamics by deep neural feedback laws
- [04705] An Operator-Learning Approach for Computational Fluid Dynamics
- [04777] Dynamic Control in Machine Learning: Geometric Interpretation of deep neural networks for Multi-Classification and Universal Approximation.
- [05167] Fourier Neural Poisson Reconstruction
- [05373] Adaptive Time Stepping in Deep Neural Networks

**[00295] Estimation problems over groups**

- [05122] Vector bundles for alignment and dimensionality reduction
- [04867] Group-robust metrics
- [04814] The sample complexity of multireference alignment and cryo-EM
- [04753] Autocorrelation analysis for cryo-EM with sparsity constraints
- [03118] Optimal Spectral Methods for Synchronization Problems
- [05181] Orthogonal Matrix Retrieval with Spatial Consensus for 3D Unknown-View Tomography

**[00296] Recent advances on two-phase flows, fluid-structure interactions, and interface problems**

- [02815] High Order Compact Finite Difference Schemes for Helmholtz Interface Problem
- [03418] Cubic Hermite splines plus correction terms: a way of adaption to the presence of singularities
- [02836] Difference Finite Element Method for 3D Steady Navier-Stokes Equations
- [03698] Finite difference method on staggered grids for Stokes-Biot problems
- [05336] Value function approximation of PDEs
- [03699] A hybrid asymptotic and augmented compact FVM for degenerate interface problem with extreme conditions
- [03531] A fast front-tracking approach for a temporal multiscale blood flow problem
- [03479] An Energy Stable Immersed Boundary Method for Deformable Membrane Problem with Non-uniform Density and Viscosity

**[00297] Wave scattering problems: numerical methods with applications**

- [02173] Fast butterfly compressed Hadamard-Babich integrators for Helmholtz equations
- [03005] Inverse wave-number dependent source problems
- [04115] The PML-method for a scattering problem for a local perturbation of an open periodic waveguide
- [03704] A PML method for signal-propagation problems in axon
- [01969] Frequency-time Green function acceleration for simulation, optimization and design
- [03041] Analysis of scattering matrix algorithm
- [04576] On the coupling schemes of finite element and boundary integral equation methods solving the acoustic/elastic scattering problems
- [03004] Fast multipole method in layered media: from Helmholtz to Maxwell's equations
- [03722] Dirac points for the honeycomb lattice with impenetrable obstacles
- [03675] Electronic Structure of Incommensurate 2D Heterostructures with Mechanical Relaxation
- [03832] Structural Symmetry and Fabry-Perot Bound States in the Continuum: A Numerical Study

**[00304] Phase transition and control of PDE models in applied sciences**

- [01375] Crowd pressure and turbulence in crowd disasters
- [01721] Traceability of Water Pollution governed by an Inverse Source Problem
- [03877] A Cucker-Smale inspired deterministic Mean Field Game with velocity interactions
- [05554] Provable convergence of blow-up time of numerical approximations for a class of convection-diffusion equations

**[00305] Computational Modeling on Biomedical Diseases**

- [00317] Role of senescent tumor cells and macrophages in building a cytokine shield in the tumor microenvironment: mathematical modeling
- [00373] Patch formation driven by stochastic effects of interaction between viruses and defective interfering particles
- [01228] Modeling about prediction and improvement of therapeutic efficacy of immune checkpoint inhibitors
- [01252] Travelling waves of a new glioma invasion model.
- [01194] The role of the autoregulation mechanism in hypertension and hypotension in humans
- [01215] Collaborative research toward data driven mathematical modeling of cancer to arrive at effective treatments
- [01334] Phase-field model of mechanical stability of blood clot

**[00306] Mathematical approaches to nonlinear phenomena with singularities**

- [04427] Crystalline inverse mean curvature flow
- [04365] Pseudo-parabolic model of grain boundary motion coupled with solidification effect
- [04655] Elliptic problems involving a Hardy potential
- [04200] Solvability of a phase-field model of 3D-grain boundary motion
- [03754] Variational models for segmentation in non-euclidian settings
- [04356] Periodic solution to KWC-type system under dynamic boundary condition

- [03968] Cahn-Hilliard equations with forward-backward dynamic boundary condition and non-smooth potentials
- [04411] Optimal control for shape memory alloys of the simplified Fr'emon model in the one-dimensional case
- [03661] Geometric convergence in regularization of inverse problems
- [04617] Numerical algorithms for optimization problems of grain boundary motions
- [04370] Temperature optimization problems governed by pseudo-parabolic model of grain boundary motion
- [04841] On well-posedness of 1-harmonic map flows

**[00307] Advanced Solver for Computational Poromechanics**

- [01387] A coupled multi-field model of dynamic poro-elasticity in anisotropic porous media
- [01468] Space-time finite element multigrid solver for fully dynamic poroelasticity
- [01676] Multiscale Dynamics in Glioblastoma Growth and Spread within the Fibrous Brain Environment
- [01820] Efficient splitting schemes for poromechanics

**[00309] Population Dynamics in Biology and Medicine**

- [01291] Exploring the effects of the latent eggs on the efficacy of Wolbachia-carrying release technique
- [01943] Mathematical models for practical application of the Sterile Insect Technique
- [01092] A generalized next generation method for the effective reproduction number
- [03871] Modelling human behavioural change during the outbreak of emerging infectious disease
- [01440] Mathematical insights of chemical and Wolbachia-based mosquito control
- [02743] ON THE ORIGIN OF COMPLEX DYNAMICS IN MULTI-STRAIN DENGUE MODELS
- [04155] Covid-19: Vaccination impact after lockdown lifting and its large fluctuations
- [03501] Optimization of Vaccination strategies on a metropolitan area
- [04326] Population Dynamics in Biology and Medicine
- [04328] Population Dynamics in Biology and Medicine
- [01337] A mathematical model to melanoma growth with macrophages and immunotherapy
- [02941] A Mathematical Perspective on Resilience and Sustainability in Climate and Biodiversity
- [01827] Potential Impacts of Mass Nutritional Supplementation on Measles Dynamics

**[00316] Dynamics of patterns and traveling waves arising from reaction-diffusion systems**

- [03601] Cross-diffusion derived from predator-prey models with two behavioral states in predators
- [00453] Weak entire solutions of reaction-interface systems
- [03042] Pulse bifurcations in a three-component FitzHugh-Nagumo system
- [05009] The Motion of Weakly Interacting Waves for Reaction-Diffusion Equations in a Cylinder
- [02140] Some Progress on the spreading properties of two-species Lotka-Volterra competition-diffusion systems
- [02366] Weak interaction between traveling wave solutions in the three-species competition-diffusion systems
- [04983] Defects in the segmented pattern for oscillated reaction-diffusion systems
- [04560] Linearized eigenvalue problems in a mass-conserved reaction-diffusion compartment model

**[00319] Robust formulations for coupled multiphysics problems – Theory and applications**

- [01558] A diffuse interface method for fluid-poroelastic structure interaction
- [01781] Parameter-robust methods for the Biot-Stokes interfacial coupling
- [02817] Robust parallel solvers in cardiac modeling
- [02934] Stochastic Galerkin mixed finite element approximation for poroelasticity with uncertain inputs
- [03195] Finite element analysis for semilinear problems in liquid crystals
- [01845] Twofold Saddle-Point Formulation of Biot Poroelasticity with Stress-Dependent Diffusion
- [03220] Finite element analysis for the Navier-Lamé eigenvalue problem
- [04279] Isogeometric solvers for derived cardiac stem cell reaction-diffusion models
- [03598] Virtual element methods for Biot-Kirchhoff poroelasticity
- [04832] Analyzing Multi-Dimensional Time-Dependent Solute Transport Models
- [03951] Unfitted finite element methods for PDEs with dynamic interfaces and boundaries
- [05346] A two-way coupled Stokes-Biot-transport model
- [04578] Conservative and robust methods for the Biot-Brinkman equations in vorticity form
- [04697] A five-field mixed formulation for stationary magnetohydrodynamic flows in porous media
- [04964] Domain decomposition solvers for problems with strong interface perturbations
- [04995] Numerical solution of the Biot/elasticity interface problem using virtual element methods
- [04946] A conforming finite element method for a nonisothermal fluid-membrane interaction
- [05072] Multipoint mixed finite elements for Biot poroelasticity using a rotation-based formulation
- [05593] Application of CutFEM to the modeling of coastal processes through vegetation

**[00322] Methodological advancement in rough paths and data science**

- [01385] A real analytic view on signatures
- [01366] PCF-GAN: generating sequential data via the characteristic function of measures on the path space
- [01336] Nyström approximation and convex kernel quadrature
- [01374] Taylor remainder estimate for rough differential equations
- [01331] Optimal stopping with signatures
- [01439] Analysis on unparameterised path space: towards a coherent mathematical theory
- [01370] On some stability results in mathematical finance via rough path theory
- [01438] Kernels Methods for Stochastic Processes
- [01994] Optimal approximation with path signatures
- [01279] Using AI to Accelerate (S)PDE Solving
- [00769] Markov Chain Cubature for Bayesian Inference

[01377] Iterated integrals of Gaussian fields and ill-posedness of heat equations

**[00323] Integrating rough paths into domain applications**

[01350] Signatures and Functional Expansions

[01349] Neural Stochastic PDEs: Resolution-Invariant Learning of Continuous Spatiotemporal Dynamics

[01332] Neural Controlled Differential Equations: The Log-ODE Method

[01297] Nowcasting with signatures

[00458] Path-Dependent Neural Jump ODEs

[00499] Signature Methods for Outlier Detection

[01312] Path Development Network with Finite-dimensional Lie Group

[01355] From CCTV video streams to inferring NO<sub>2</sub> emissions at city-scale

[01359] Addressing bias adversarially in online learning.

[01353] Improving Training of Neural CDEs

[03470] From MMD-Regime detection to MMD-Generative Models with Applications

[01236] Capturing Graphs with Hypo-Elliptic Diffusions

**[00324] Minisymposium on Combinatorial Reconfiguration**

[04748] Invitation to Combinatorial Reconfiguration

[04759] Geometric algorithms for reconfiguring modular robots

[05218] Toric Promotion and Permutoctic Promotion

[04747] Triangulations of cyclic polytopes through the lens of reconfiguration

**[00336] Recent advances in Optimization methods with applications**

[02720] HABITAT LOSS AND COOPERATIVE HUNTING ON A THREE-SPECIES TROPHIC SYSTEM

[02816] Modeling of impulsive perturbations by generalized fractional differential equations

[02710] Necessary conditions to optimize functionals involving a generalized fractional derivative

[02725] Herglotz's Variational Problem involving distributed-order fractional derivatives with arbitrary kernels

**[00340] New trends in phase fields: theory & applications**

[04343] Energy stability of variable step higher order ETD-MS scheme for gradient flows

[04034] Energy Dissipation of Time-Fractional Phase-Field Equations: Analysis and Numerical methods

[02973] A Spectral Element in Time Method for Nonlinear Gradient Systems

[02987] Energy stability and error analysis of high-precision algorithms for two-phase incompressible flows

[03070] NONLOCAL CAHN-HILLIARD TYPE MODEL FOR IMAGE INPAINTING

[03100] A Variety of Gradient Flows: Modeling and Numerical Methods

**[00341] Graph Coloring**

[02669] Flows and coloring of triangle-free graphs on surfaces

[02782] Alon-Tarsi number of planar graphs

[02488] Edge-colourings, hamiltonian cycles, and a problem of Kotzig

[03108] Coloring Graphs with Forbidden Minors

**[00342] Localized waves in nonlinear discrete systems**

[00658] Existence of multi-pulse discrete breathers in Fermi-Pasta-Ulam-Tsingou lattices

[01557] Spectral properties of nonlinear excitations in semiclassical systems with charge transport

[01269] Nonlinear waves in multistable mechanical metamaterials

[01230] Soliton billiards

[00812] Universality Classes for Nonlinear Wave Thermalization

[01278] Numerical experiment on nonlinear localized oscillation propagating in a mass-spring chain

[01274] Moving Intrinsic Localized Modes Created by Transforming Wavenumber-frequency Spectrum of a Static Intrinsic Localized Mode in FPUT-NKG Mixed Lattices

[00992] Structure of pairwise interaction symmetric lattice for moving discrete breather

**[00345] Recent Developments for High-frequency Waves and Tomography**

[03696] Learning based on data and numerical solutions for differential equations

[01633] Butterfly-compressed Hadamard-Babich Integrator for High-Frequency Helmholtz and Maxwell Equations in Inhomogeneous Media

[02074] Development and Analysis a higher-order numerical method for Helmholtz equation with high wave number

[02172] Fixed Angle Inverse Scattering For Velocity

[02057] Eulerian PDE methods for complex-valued eikonalns in attenuating media

[01878] Uniformly convex neural networks and iterated network Tikhonov (iNETT) method

[03580] Linearized Inverse Potential Problems at a High Frequency

[03600] An Embedding Method for Hyperbolic Conservation Laws on Implicit Surfaces

**[00353] Interpretable constrained tensor decompositions: models, algorithms, efficient implementations and applications**

[03825] Implicit balancing in penalized low-rank approximations

[02791] Hierarchical and neural nonnegative tensor factorizations

[03781] Nonnegative canonical tensor decomposition with linear constraints: nnCANDELINC

[04213] Joint Data Fusion and Blind Unmixing using Nonnegative Tensor Decomposition

[04776] A quadratically convergent proximal algorithm for nonnegative tensor decomposition

[03079] PARAFAC2-based coupled matrix and tensor factorizations with constraints

[03791] Constrained Tucker Decompositions and Conservation Principles for Direct Numerical Simulation Data Compression

[03819] Incremental Nonnegative Tucker Decomposition with Block-coordinate Descent and Recursive Approaches

- [05162] Speeding up Nonnegative Low-rank Approximations with Parallelism and Randomization.
- [03142] A probabilistic nonnegative tensor factorization method for tumor microenvironment analysis
- [03182] Scalable symmetric Tucker tensor decomposition
- [02021] A tensor factorization model of multilayer network interdependence

**[00356] Recent progress in variational problems with nonlocality**

- [03768] Nonlocal capillarity theory
- [03751] Skyrmion theory in magnetic thin films: the role of non-local magnetic dipolar interaction
- [05516] Long-range phase transition equations
- [04003] A distributional approach to nonlocal curvature motions
- [03830] The elastica functional as the critical Gamma-limit of the screened Gamow model
- [04447] Minimisers of anisotropic Coulomb energies in 3d
- [03755] Minimal partitions for local and nonlocal energies
- [03839] Asymptotics of phase field models for crystal defects

**[00357] Topics at the Interface between Applied mathematics and Microeconomics**

- [01659] Commitment games with mutual interferences
- [01666] Equilibria in a spatial competition with uninformed consumers
- [01655] Gradient flows in travelers' visitation network: comparison with centrality indices
- [01678] Information Design and Pre-trade Investment

**[00372] Recent advances on computational wave propagation**

- [01429] Analysis and simulation of carpet cloak model with metamaterials
- [01639] Edge elements on nonaffine quadrilateral and hexahedral grids for Maxwell eigenproblem
- [01856] Deriving consistent surface fields for compatible FETD discretizations of Maxwell's equations
- [01860] FDTD Method With Explicit Non-Iterative and Second Order Treatment for Kerr Nonlinearities
- [02077] Harnessing the Power of Exascale Computing for Microelectronics Modeling
- [02080] Simulating Time Domain Electromagnetic Waves on a Differentiable Programming Platform
- [02117] Iterative two-level algorithm for nonsymmetric or indefinite problems
- [01863] Analysis and application of FEMs for Ziolkowski's PML model
- [02737] Highly Efficient Iterative Method with High Order ABC for Acoustic Scattering
- [02916] The effect normal electric fields on the flow structure beneath waves

**[00378] Mathematical Methods in System Reliability**

- [01347] Domination and multistate systems
- [01419] Mathematical analysis of the reliability of stable systems
- [01422] Algebraic probability: the case of system reliability
- [01425] Algebraic analysis of importance measures of coherent systems
- [01455] New exactly solvable architecture for system reliability and safety
- [01469] Application of Logic Differential Calculus in Reliability Analysis
- [03092] Stochastic comparisons of coherent systems with active redundancy at component level and system level

**[00379] Numerical techniques for coarse-graining, model reducing and simulation of complex physical systems**

- [02156] Ahyper-reduced MAC scheme for the parametric Stokes and Navier-Stokes equations
- [02166] Hybrid Projection Methods for Solution Decomposition in Large-scale Bayesian Inverse Problems
- [02484] A reduced basis method for the parametrized Monge-Ampere equation
- [04068] Novel Reduced Basis Method for Radiative Transfer Equation
- [03752] Large Deviations for Model Coarse Graining
- [03592] Mean curvature flow as the limit of a spin system
- [04679] Model reduction methods for non-reversible multiscale dynamics: a comparison
- [04002] Model Reduction using the Koopman Operator
- [04693] Machine-learning-based spectral methods for partial differential equations
- [03852] Optimal control for fractional order equations
- [04163] Multi-Resolution and FVM inspired Neural Network (MuRFiV-Net) for PDE prediction

**[00382] Stochastic control and stochastic analysis in finance and insurance**

- [02210] Lévy bandits under Poissonian decision times
- [02144] Optimal Consumption with Loss Aversion and Reference to Past Spending Maximum
- [02873] On the Entropy martingale optimal transport
- [02785] Functional convex order for the McKean-Vlasov equation
- [0, T]} and  $\{\nu_t\}_{t \in [0, T]}$ . For a convex functional  $G(X)$ , defined on the product space involving the path space and its marginal distribution space, we obtain  $\mathbb{E}[G(X)] \leq \mathbb{E}[G(Y)]$ , where  $\mathbb{E}$  is the expectation with respect to the law of the process  $(Y_t)_{t \in [0, T]}$ .
- [0, T]}  $\leq \mathbb{E}[G(Y)]$ , under appropriate conditions. This presentation also includes two applications of the convex order result to mean-field control and mean-field games.
- [03167] Incentive to shape equilibria in double auction markets
- [04566] On time-consistent equilibrium stopping under aggregation of diverse discount rates
- [02775] CONVERGENCE OF POLICY IMPROVEMENT FOR ENTROPY-REGULARIZED STOCHASTIC CONTROL PROBLEMS
- [03347] Continuous time q-learning for McKean-Vlasov control problems

- [02892] Skew Brownian Motion with Two-Valued Drift
- [02928] Pathwise uniqueness of SDEs driven by stable processes
- [05583] Mean field portfolio games
- [03375] A mean-field version of Bank--El Karoui's representation of stochastic processes
- [00384] Origami Engineering (1/2)**
  - [01360] Farthest point map on the double cover of a parallelotope
  - [01518] Deployable earwig fan dome with the algorithmic design tool
  - [01519] Geometry and mechanics of molting in snakes and caterpillars
  - [01523] Linear transformation of crease pattern boundaries preserving internal graph isomorphisms
  - [01571] Laboratory-scale Workshop for Enhancing Designability of Origami Cores
  - [01618] Strip folding as Boolean matrix algebra and its Categorical Meanings
  - [02328] Application of the proposed method to a transport origami box
  - [01536] Refoldability between polyhedra
  - [05407] Optimal Simple Fold-and-Cut of a Polygonal Line
  - [02335] Geometrical Comparison of Two kinds of Pairing Origami Polyhedron and Their Application to Beverage Containers
- [00385] Origami Engineering (2/2)**
  - [01402] Solitons in Origami / Kirigami Tessellations and Their Underlying Dynamical Systems
  - [01403] Macroscopic Behavior of Kirigami Tessellations with Contact Surfaces
  - [01432] Miura fold bending in two directions and their combination
  - [01526] Development study of foldable and portable comfortable acoustic space
  - [01562] A remark on the foldability of non-simply connected paper
  - [05414] Origami Structures and Materials: Energy Absorption and Impact Mechanics
  - [02536] Platonic solids-based optimization for kirigami honeycomb fabrication of complex structures
  - [02542] Development of beautifully foldable PET bottles
- [00389] Randomized methods for solving linear systems and eigenvalue problems**
  - [03670] Making the Nystrom method highly accurate for low-rank approximations
  - [04016] Superfast iterative refinement of Low Rank Approximation of a Matrix
  - [00881] Relaxation in low-rank updates of Schur complement preconditioners in fluid flow problems
  - [00530] Randomized low-rank approximations beyond Gaussian random matrices
  - [04523] Are randomized NLA algorithms numerically stable?
  - [05547] Randomized orthogonalization process
  - [04952] A robust randomized indicator method for accurate symmetric eigenvalue detection
  - [05321] The Adversarially Robust Generalized Eigenvalue Problem
  - [03799] Stochastic Gradient Descent with Conjugate Gradient-style Momentum
  - [01342] Robust randomized preconditioning for kernel ridge regression
  - [01305] Structured matrix recovery using randomized matrix-vector products
- [00390] Recent Advances in Machine Learning Theory and Applications**
  - [03668] Learning through empirical gain maximization
  - [01357] SKELETAL BASED IMAGE PROCESSING FOR CNN BASED IMAGE CLASSIFICATION
  - [01023] Total stability of kernel methods and localized learning
  - [01397] Learning Ability of Interpolating Convolutional Neural Networks
  - [03542] Classification with Deep Neural Networks
  - [03729] Robust Deep Learning with Applications
- [00391] Recent Advances in Multiscale Transforms for Image Analysis**
  - [01735] Multiscale monogenic image representations using Poisson kernels
  - [02090] Image Interpolation Technique by the PCA of the Gradient Distribution
  - [02079] Improvement of coding procedures for Haar transform-based lossy image compression
  - [02086] Edge enhancement with directional wavelet transform
- [00400] Bilevel optimization in machine learning and imaging sciences**
  - [03653] Fixed-Point Automatic Differentiation of Forward--Backward Splitting Algorithms for Partly Smooth Functions
  - [05289] A framework for bilevel optimization that enables stochastic and global variance reduction algorithms
  - [03309] Bilevel Optimization with a Lower-level Contraction: Optimal Sample Complexity without Warm-Start
  - [02768] Bilevel subspace optimisation in heterogeneous clustering for cryo-EM
  - [05645] Test like you train in implicit deep learning
- [00404] Large-Scale Eigenvalue Computations and Optimization**
  - [03074] Consistent Estimation Using SVD for a Linear Regression Model
  - [04078] Fast optimization of eigenvalues for frequency-based damping of second-order systems
  - [02304] Rectangular multiparameter eigenvalue problems
  - [04501] Simultaneous diagonalization and new bounds on shared invariant subspaces
  - [03188] Estimation of the dominant poles of a large-scale descriptor system
  - [03212] Subspace Methods for Nonlinear Eigenvalue Problems
  - [05296] Optimizing orthogonality in large-scale tensor networks
  - [05462] Linearizability of eigenvector nonlinearities
- [00410] Recent advances in Bayesian optimal experimental design**
  - [04376] A transport map approach for Bayesian optimal experimental design
  - [04957] Accelerating A-Optimal Design of Experiments Using Neural Networks

[05059] Stability of Bayesian optimal experimental design in inverse problem

[05080] Quasi-Monte Carlo methods for Design of Experiment

**[00413] Numerical Methods for Dispersive PDEs and Applications**

[05510] Numerical studies of two regularized versions of the cubic NLS

[05557] Dirac equations for the modeling of electron dynamics on strained graphene surfaces

[02732] Low regularity exponential-type integrators for the "good" Boussinesq equation

[04017] Computational methods for stationary states of nonlinear Schrödinger/Gross-Pitaevskii equations

[05499] Scattering and uniform in time error estimates for splitting method in NLS

[05587] Resonances as a computational tool

[01752] Error estimates of numerical methods for the nonlinear Schrödinger equation with low regularity potential and nonlinearity

**[00418] Nonlinear PDE: beyond the well-posedness theory**

[01572] Hessian Riemannian flows in mean-field games

[02413] Homogenization of Reactions in Random Media

[02535] Continuum limit of dislocations with annihilation in one dimension

[04586] Quantitative periodic homogenization of a front propagation model in dynamic environments

**[00420] Painlevé equations, Applications, and Related Topics**

[04296] The Identification Problem for Discrete Painlevé Equations

[04597] Orthogonal polynomials and discrete Painlevé equations on the  $D_5^{(1)}$  Sakai surface

[03019] Orthogonal polynomials, Schur flow and Painlevé equations

[04527] Symmetries of discrete Nahm systems and Normalizers in Coxeter groups

[04366] On the bilinear equations of the Painlevé transcenders

[04932] Large-degree asymptotics of Generalized Hastings-McLeod functions

[04515] Spaces of initial values for equations with the quasi-Painlevé property

[02754] On the (quasi-)Painlevé equations

[03574] A dynamical systems approach to map enumeration

[03010] An affine Weyl group action on the basic hypergeometric series

[03311] On the growth properties of some families of birational maps

[05042] Laguerre (q-Laguerre) Weight Recurrence and Geometric Theory of Painlevé equations

[04054] Folding transformations for q-Painlevé equations

[04739] Laguerre (q-Laguerre) Weight Recurrence and Geometric Theory of Painlevé equations

**[00421] When random comes to the rescue of numerical computation**

[02748] The computer arithmetic new deal: AI is pushing the frontier

[01590] New stochastic rounding modes for numerical verification

[04711] Stochastic rounding as a model of round-to-nearest

[03452] VPREC to analyze the precision appetites and numerical abnormalities of several proxy applications

**[00426] Variational methods for thin structures and free-boundary problems**

[03469] On the Kirchhoff-Plateau problem: critical points and regularity

[02176] On Stationary Points of Polyconvex Functionals

[04199] Minimization of the Canham-Helfrich within generalised Gauss graphs

[03181] A capillarity theory approach to the analysis of soap films

[04117] Stable Möbius bands obtained by isometrically deforming circular helicoids

[02967] Rectifiability for flat singularities of higher codimension area minimizers

[03455] Interior regularity for stationary two-dimensional multivalued maps

[03306] Transport of currents and geometric Rademacher-type theorems

[02741] Long time behavior and stability of surface diffusion flow

[03626] Graphical solutions to one-phase problems

[04656] Regularity of the optimal shapes for a class of integral functionals

[04579] Min-max minimal surfaces with contact angle conditions

**[00432] Empirically Driven Deep Learning Theory**

[02983] How different optimizers select the global minimizer in deep learning

[03263] A Law of Data Separation in Deep Learning

[03057] Neural Collapse in Deep Learning

[03168] Memorization-Dilation: A Novel Model for Neural Collapse in Deep Neural Network Classifiers

[04878] Understanding Deep Learning Through Optimization Geometry

[04289] Feature Learning in Two-Layer Neural Networks

[03006] On the Implicit Geometry of Deep-net Classifiers

[05316] Does the loss function matter in overparameterized models?

**[00435] Multiscale Numerical Methods for Complex Fluids**

[05277] Multi-Physics Simulations of Flow, Friction, and Reactions in Solid/Liquid Interface

[02346] Numerical modeling of viscoelastic flows with high elasticity

[02354] DPD Simulation of Ultrasound Propagation through Liquid Water

[04595] Machine-Learning for Accelerated Multi-Scale Polymer Flow Simulations

[03437] Simulation of micro-scale particulate motion in gases

[03686] Synchronized Molecular-Dynamics simulation of the thermal lubrication of an entangled polymer melt

[03368] Simulation of multiphase flows based on Lagrangian methods

- [03717] Lagrangian Heterogeneous Multiscale Methods: A generalized multiphysics model for complex fluids with memory
- [05555] Moisture-induced weakening of adhesion between polymers and metals
- [03509] Modelling and Simulation of Capillary Origami in Three Dimensions
- [04590] Multiscale simulation of a polymer melt flow between two coaxial cylinders under nonisothermal conditions
- [05592] Flow-type dependent rheologies and multiscale simulations

**[00436] Coupled dynamical systems: from data analysis to biomathematics**

- [03097] Fractal dimension of multidimensional biological recordings
- [03895] Lyapunov-like characterization of ghost and weak attractors in complex dynamical systems
- [03442] Flip-flip bifurcations in mathematical cardiac systems with and without symmetry
- [03235] Generation of early afterdepolarizations in cardiomyocytes: Fast-slow and bifurcation analysis

**[00437] Climate Risks: From Modelling to Applications**

- [01677] Optimal ecological transition path of a credit portfolio distribution, based on Multidate Monge-Kantorovich formulation
- [01674] Optimal Dynamic Contracts and Environmental Pollution
- [05305] Optimal Impact Portfolios with General Dependence and Marginals
- [01585] Using NLP to Analyze Corporate Communication
- [01328] When Green Investors Are Green Consumers
- [01612] Bridging Shared Socioeconomic Pathways of GHG Emission and Credit Risk
- [01683] On some initial climate change impact models in actuarial science
- [05370] Optimal carbon tax in the Golosov et al. 2014 DGSE central planning model

**[00441] Intersection between financial economics and optimal control**

- [05612] Asset Pricing with Misallocation
- [03797] An optimal consumption and investment problem for general factor models : Epstein-Zin recursive utility case.
- [05413] Patience is a virtue: optimal investment in the presence of limit order book
- [05411] Why is Cash U-Shape in Firm Size?
- [02868] Debt Maturity Management
- [05611] Nonlinear Dependence and Households' Portfolio Decisions over the Life Cycle
- [04014] Dynamic Equilibrium with Insider Information and General Uninformed Agent Utility

**[00444] Complex Systems: Advances in Theory and Applications**

- [01282] Time Series Analysis with Machine Learning
- [01306] On constructing directed networks from multivariate time series
- [05563] Optimal network synchronization and a higher-order topological approach
- [01273] Evaluating the Network Robustness: A Convolutional Neural Network Approach
- [01264] Adaptive Finite-Time Output Consensus for Fractional-Order Complex Networks With Multiple Output Derivative Couplings
- [01255] Optimizing 3D Complex Networks on chip
- [01268] Machine Learning for Detecting Internet Traffic Anomalies
- [01280] Model for estimating unconfirmed COVID-19 cases and multiple waves of pandemic progression

**[00448] Particle based methods**

- [02827] Constrained sampling
- [03107] Subsampling in ensemble kalman inversion
- [03842] Ensemble Inference Methods for Models with Noisy and Expensive Likelihoods
- [04379] Projected ensemble data assimilation
- [04587] Alternatives to Monte Carlo based sampling and high dimensional integration
- [05018] Mixtures of Gaussian Process Experts with SMC<sup>2</sup>
- [05073] Eulerian calibration for stochastic transport models
- [05209] Can possibility theory help with uncertainty quantification for neural networks?

**[00449] Atomistic simulations in the exascale era**

- [01608] Quantum Materials Simulations at the Nexus of Exascale Computing, Artificial Intelligence, and Quantum Computing
- [01950] Large scale quantum chemistry with Tensor Processing Units
- [02042] Quantum molecular dynamics using Tensor cores
- [02949] Recent algorithmic improvements in parallel long-time molecular dynamics
- [03771] Adaptive parareal method for the simulation of atomistic defects
- [04027] Fast, Accurate and Large-scale Ab-initio Calculations for Materials Modeling
- [04848] The Chunks and Tasks Matrix Library
- [05282] From Langevin dynamics to kinetic Monte Carlo: mathematical foundations of accelerated dynamics algorithms
- [05409] Quantum-Mechanical Shadow Born-Oppenheimer Molecular Dynamics for Distributed Computing
- [05380] Compressing, resampling and forecasting atomic simulations with descriptor vectors
- [05479] Structure modeling with large-scale DFT and machine-learning methods

**[00455] Recent Development of Theory and Algorithms of Scientific Machine Learning**

- [05474] Monte Carlo neural networks: Stochastic gradient descent learns random variables
- [01329] Deep adaptive basis Galerkin method for evolution equations
- [01635] Identifying reaction channels via reinforcement learning
- [03340] Finite Expression Methods for Discovering Pyhsical Laws from Data
- [03345] Approximation Theory for Sequence Modelling

- [03154] Finite Expression Method: A Symbolic Approach for Scientific Machine Learning
- [01880] Discretization Invariant Operator Learning for Solving Inverse Problems
- [03159] Deep Adaptive Basis Galerkin Method for Evolution Equations
- [03467] Multi-scale Neural Networks for High Frequency Problems in Regressions and PDEs
- [05449] Implicit bias in deep learning based PDE solvers

**[00462] Mathematical and applicable studies on quantum walks**

- [01759] The Ihara expression of graph zeta functions
- [02778] Topological stability of quantum walks and related
- [03296] Spectral mapping theorem for quantum walks on graphs
- [05096] The Segawa-Suzuki spectral mapping theorem, revisited
- [03456] Resonance expansion for quantum walks
- [04207] Spectral scattering theory for quantum walks
- [04051] Quantum Walk-Based Maze-Solving with Absorbing Holes
- [03689] Distinguishability and Complexity in Non-Unitary Boson Sampling Dynamics

**[00465] Linear and Non-linear Approximation of Curves and Surfaces**

- [01862] Stable nonlinear inversion : a general framework for interface reconstruction from cell-average
- [02134] Adaptive Multi-Quadric Interpolation: Applications in Image Compression.
- [01772] Reconstructing a Digital Elevation Model from C2 quasi-interpolation
- [01766] Low-degree quasi-interpolation in the Bernstein basis
- [01326] A Nonlinear B-spline quasi-interpolation method,
- [01853] Edge adaptive schemes and machine learning for image super-resolution
- [01411] Univariate subdivision schemes based on local polynomial regression
- [01410] Linear and nonlinear approximation rules arising from optimal denoising
- [01560] A totally C^2 quartic splines defined on mixed macro-structures
- [01502] Construction of quadratic and cubic orthogonal wB-spline wavelets
- [01492] Algebraic Hyperbolic spline interpolation by means of integral values.

**[00467] Volatility modeling in finance**

- [05137] Volatility is (Mostly) Path-Dependent
- [05626] The 4-Factor Path-Dependent Volatility Model
- [01960] A theoretical analysis of Guyon's toy volatility model
- [05614] Prediction through Path Shadowing Monte-Carlo
- [04506] Understanding how market impact shapes rough volatility
- [04065] Pricing in affine forward variance models
- [02829] The rough Hawkes Heston model
- [05086] Recent advances on rough volatility
- [04764] Does the Term-Structure of Equity At-the-Money Skew Really Follow a Power Law?
- [04899] Fast exact joint S&P 500/VIX smile calibration in discrete and continuous time
- [03758] Joint calibration to SPX and VIX options with signature-based models
- [03638] Neural Joint SPX/VIX Smile Calibration

**[00468] Stochastic Modelling in Finance<sup>U.S.E.P.</sup>**

- [01313] Portfolio optimization in the family of 4/2 stochastic volatility models.
- [01486] Parrondo's paradox and financial applications
- [01304] Optimal portfolio analysis on finite and small-time horizons
- [01292] Stochastic Modelling of Big Data in Finance

**[00471] Recent Advancements in Electrical Impedance Tomography**

- [04879] A Multithreaded Implementation of the D-bar Algorithm for 2D Functional EIT Imaging
- [02729] New insight into EIT reconstruction using virtual X-rays
- [04009] Combining electrical impedance tomography and machine learning for stroke classification
- [03129] Recent developments on integral equation approaches for Electrical Impedance Tomography
- [04744] Monitoring of hemorrhagic stroke using Electrical Impedance Tomography
- [04874] Exploration of deep generative modelling approaches to electrical impedance tomography
- [04904] Fast CGO-based absolute reconstructions for 3D EIT
- [05054] Use of reference measurements in electrical tomography

**[00475] Variational methods and periodic solutions in the n-body problem**

- [04108] Regularizing Fuel-Optimal, Multi-Impulse Trajectories with Second-Order Derivatives
- [04642] Floquet Mode-Based Transfer between Halo Orbits Using Solar Sails
- [04549] Low-energy Transfer to the Earth-Moon Periodic Orbit: CubeSat Application
- [04028] Transfer between Resonances via Lobe Dynamics in the Standard Map
- [03973] Distance estimates for action-minimizing solutions of the n-body problem
- [04970] Some progress on the N-center problem by variational methods
- [04318] Periodic solutions bifurcated from the figure-eight choreography: non-planar eight and non-symmetric eight
- [04797] Variational structures for infinite transition orbits of monotone twist maps
- [03812] Periodic and homo/heteroclinic solutions of the restricted three-body problem
- [04714] Existence of transit orbits in the restricted three-body problem
- [03894] regularizable collinear periodic solutions in the n-body problem with arbitrary masses
- [03430] Braids and periodic solutions of the planar N-body problem

**[00479] Advances in clinically-driven AI image reconstruction and processing**

- [05254] The impact of model-based ML driven CT reconstruction on tumor segmentation and clinical diagnosis
- [03919] Bringing research advances in imaging sciences into the clinic
- [02867] Spectral Normalisation of Depthwise Separable Convolutions for Medical Applications
- [05266] Mice PET/CT Dataset Augmentation using a 3D Single Image GAN

**[00484] Matrix Analysis and Applications**

- [01267] Combinatorial Perron Parameters and Classes of Trees
- [01379] Poset matrices and associated algebras
- [01266] Majorization orders for  $(0, \pm 1)$ -matrices
- [00830] The ranks and decompositions of quaternion tensors
- [03621] Log-majorization and inequalities of power means
- [00868] Matrix Problems in International Economics
- [01404] Spectral inequalities for Kubo-Ando and Heinz means
- [00800] Limit of the induced Aluthge transformations
- [01263] Geometric inequalities for contraction matrices
- [01307] The generalized quaternion matrix equation
- [01222] Some new results on matrix and tensor equations
- [01920] Matrix inequalities and properties of means on positive definite matrices
- [05621] How to check D-stability: a simple determinantal test

**[00488] Eigenvector-Dependent Nonlinear Eigenvalue Problems: Theory, Algorithms and Applications**

- [03905] A Self-Consistent-Field Iteration for OCCA
- [04633] Mathematical Analysis and Numerical Approximations of Density Functional Theory Models for Metallic Systems
- [05119] Convergence of SCF Iteration for Eigenvector-dependent Nonlinear Eigenvalue Problems
- [04225] Geometric inexact Newton method for generalized singular values
- [05381] Nonlinear spectral graph theory: an overview of graph properties
- [05445] Solving Non-Convex Problems without Relaxation: Unexpected Usefulness of NEPv on Optimization Theory
- [05390] Trace Minimization Principles on Matrix Manifolds
- [05272] Bound states in the continuum for a class of infinite matrices

**[00496] Recent development in Quantum Simulation and Stochastic Methods**

- [02786] Orthogonalization and Orthogonalization-free Algorithms
- [01872] Frozen Gaussian Sampling for mixed quantum-classical dynamics
- [02280] The Random Feature Method for Time-dependent Problems
- [02728] Numerical methods for disordered NLS
- [02819] Asymmetric transport and topological invariants
- [02812] Asymmetric transport computations in Dirac models of topological insulators
- [01869] Quantum Orbital Minimization Method for Excited States Calculation on Quantum Computer
- [02283] Bloch decomposition based method for Schrödinger equation with random inputs
- [02028] On Quantum Speedups for Nonconvex Optimization via Quantum Tunneling Walks
- [02822] Quantum dynamics simulation and its application to Hamiltonian learning

**[00497] Advances in numerical methods for nonlinear optics**

- [03183] High-Order Accurate Approaches for Maxwell's Equations with Nonlinear Active Media on Overlapping Grids
- [02203] Energy stability and active Q-factor control in numerical models of nonlinear electromagnetic resonance effects
- [02291] Energy stable finite element method for nonlinear Maxwell's equations
- [03742] High Order Energy Stable FDTD Methods for Maxwell Duffing models in Nonlinear Photonics
- [05175] Local time-integration for wave equations
- [02186] Discontinuous Galerkin Time-Domain methods for nonlinear active media on unstructured grids

**[00498] Approximation and modeling with manifold-valued data**

- [05470] Implicit integration along the low-rank manifold for stiff and nonlinear equations
- [04268] Stochastic modeling of model uncertainties through Riemannian reduced-order representations
- [05113] On approximation and representation of manifold-valued functions
- [05093] Multivariate Hermite Interpolation On Riemannian Manifolds
- [01628] Approximations and learning in the Wasserstein space
- [05075] On multiscale quasi-interpolation of scattered scalar- and manifold-valued functions
- [03824] The de Casteljau algorithm on symmetric spaces
- [04608] Structure-preserving Model Order Reduction on Manifolds
- [03709] The Difference of Convex Algorithm on Riemannian Manifolds
- [02950] Symplectic model order reduction via Riemannian optimization
- [05465] Hirotugu Akaike's Analysis of Gradient Descent: 70 years later

**[00505] Structured matrices with applications in sciences and engineering**

- [02264] Reciprocal Matrices, Ranking and the Relationship with Social Choice
- [01723] A matrix approach to the study of efficient vectors in priority setting methodology
- [00811] Singular matrices whose Moore-Penrose inverse is tridiagonal.
- [03060] Spectral geometric mean versus geometric mean by generalized Kantorovich constant
- [05539] Bundles of matrix pencils under strict equivalence
- [05542] Row completion of polynomial matrices
- [01819] Computational Techniques for the Mittag-Leffler Function of a Matrix Argument

[02170] A reduction algorithm for reconstructing periodic pseudo-Jacobi matrices

[05469] A Low-Cost Algorithm to Determine Orbital Trajectories

**[00506] Inverse Problems for Anomalous Diffusion**

[01356] Coefficient identification space-fractional equation with Abel type operators

[04481] Inverse problems for simultaneous determination of several scalar parameters and source factors in anomalous diffusion equations

[03427] Parameter inverse problem for coupled time-fractional diffusion systems

[04183] Identification of potential in diffusion equations from terminal observation

[04736] Classical Unique Continuation Property for Time Fractional Evolution Equations

[02704] The Calderón problem for nonlocal parabolic operators

[02699] Inverse Problems for Subdiffusion from Observation at an Unknown Terminal Time

[04403] Numerical Recovery of Multiple Parameters from One Lateral Boundary Measurement

[04435] Long-Short time asymptotic estimates for time-fractional diffusion-wave equation

[04612] Numerical identification of conductivity in (sub)diffusion equations from terminal measurement

**[00507] Stochastic Dynamical Systems and Applications**

[04264] Three-dimensional numerical study on wrinkling of vesicles in elongation flow

[04452] Energetic Variation associated with nonlinear Schrödinger equations with Anderson Hamiltonian

[04457] Macroscopic approximation for stochastic N-particle system with small mass

[04557] Effective wave factorization for a stochastic Schrodinger equation

[04528] Approximation of nonlinear filtering for multiscale McKean-Vlasov stochastic differential equations

[04629] On the WKB approximation of confluent hypergeometric systems

[04570] Global stability of stochastic functional differential equations

[04648] Averaging principle for slow-fast systems of stochastic PDEs with rough coefficients

[04756] Mean Asymptotic Behavior for Stochastic Kuramoto-Sivashinsky Equation in Bochner Spaces

[04325] The Poisson Equation and Application to Multi-Scale SDEs with State-Dependent Switching

[04954] A stochastic fractional Schrodinger equation with multiplicative noise

[05083] The most probable dynamics of receptor-ligand binding on cell membrane

**[00509] Recent developments in stochastic optimization**

[00650] Random activations in primal-dual splittings for monotone inclusions with a priori information

[01376] New results on Carathéodory integral functions, applications to stochastic optimization

[03790] Adaptive partition-based method for 2-stage stochastic linear programming

[03978] Multistage optimization of a partially observed petroleum production system

[05112] Convex stochastic optimization

**[00517] Numerical Modelling of Highly Flexible Structures for Industrial Applications**

[02070] Augmented Lagrangian contact formulation of the 2D Euler elastica

[02324] The velocity-based formulation for static and dynamic analysis of non-linear three-dimensional frames

[02419] Half-explicit time integration of constrained mechanical systems on Lie groups

[02155] Frequency-dependent damping as forcing on multisymplectic integrators

**[00521] Recent advances on non-convex optimization in inverse problems, imaging and machine learning**

[02446] Convergence rate analysis of a Dykstra-type projection algorithm

[04336] Critical points of the projection onto the set of low rank tensors

[05256] Nonconvex Semi-algebraic Optimization: From Exact to Convergent Conic Program Relaxations

[01258] Global convergence of the gradient method for functions definable in o-minimal structures

[04681] Convergence theory for mean-field optimization methods

[03322] Convergence Theorem for Deep Neural Network with ReLU Activation

[05068] Theoretical and practical applications of signomial rings to polynomial optimization

[04380] Proximal methods for nonsmooth and nonconvex fractional programs: when sparse optimization meets fractional programs

[03321] Error bounds based on facial residual functions

[02798] Doubly majorized algorithm for sparsity-inducing optimization problems with regularizer-compatible constraints

[04271] Differentiating Nonsmooth Solutions to Parametric Monotone Inclusion Problems

[01315] Optimal Neural Network Approximation of Wasserstein Gradient Direction via Convex Optimization

[01537] Data-informed deep optimization

[02734] Continuous Newton-like Methods featuring Inertia and Variable Mass

[01611] Inertial quasi-Newton methods for monotone inclusion

[05250] Extrapolated Proximal Algorithms for Nonconvex and Nonsmooth Min-max problems

[05578] Global stability of first-order methods for coercive tame functions

**[00523] Implicit methods for hyperbolic problems and their extensions and applications**

[04131] Semi-implicit schemes for a convection-diffusion-reaction model of sequencing batch reactors

[01691] High resolution well-balanced compact implicit numerical scheme for numerical solution of the shallow water equations

[01692] Numerical solution of scalar hyperbolic problems using the third order accurate compact implicit scheme

[05425] High-fidelity multiderivative time integration for compressible flows

[01684] Implicit and semi-implicit well-balanced finite volume methods for general 1d systems of balance laws

[01665] SHALLOW-WATER MODEL: IMPLICIT FULLY WELL-BALANCED METHODS IN THE LAGRANGE-PROJECTION FRAMEWORK

- [01664] Hyperbolic systems with stiff relaxation: asymptotic-preserving and well-balanced schemes
- [01673] MIRK methods and applications in RRMHD and neutrino transport equations
- [03904] Implicit-explicit schemes for Cahn-Hilliard-Navier-Stokes equations

**[00524] Lie Symmetries, Solutions and Conservation laws of nonlinear differential equations**

- [02723] Conservation laws and variational structure of damped nonlinear wave equations
- [03330] Constructing mass-conserving cnoidal wave solutions for the KdV equation
- [04290] Conservation laws and symmetries of a Generalized Drinfeld-Sokolov system
- [02959] Lie symmetry analysis of flow and pressure inside horizontal chamber
- [03457] Closed-form solutions and conservation laws of the fifth-order strain wave equation in microstructured solids
- [02308] Symmetry solutions and conservation laws of the derivative nonlinear Schrodinger equation
- [03449] Lie symmetry analysis of new 3-D fifth-order nonlinear Wazwaz equation
- [03451] Lie group analysis of the nonlinear 3D KP-BBM equation
- [04488] Integrable equations and Riemann-Hilbert problems
- [04064] A study of 3D generalized nonlinear wave equation in fluids
- [04126] Burgers' nth Partial Differential Equation Hierarchy
- [03471] Nonclassical Potential Symmetries for the transient heat transfer equation

**[00528] High order and well-balanced methods and stability analysis for non-linear hyperbolic systems**

- [01682] High order well-balanced finite volume and discontinuous Galerkin schemes for a first order hyperbolic reformulation of the coupled Einstein-Euler system in 3+1 general relativity
- [01699] Numerical approximation of non-convex relativistic hydrodynamics
- [01720] Recovering primitive variables in special relativistic hydrodynamics
- [01290] Well-Balanced High-Order Discontinuous Galerkin Methods for Systems of Balance Laws
- [01687] Structure preserving high order discontinuous Galerkin schemes for general relativity
- [01663] Multidimensional approximate Riemann solvers for hyperbolic nonconservative systems
- [01841] A fully-well-balanced hydrodynamic reconstruction
- [01690] A well-balanced scheme for landslide models

**[00529] Numerical approximation of geophysical flows**

- [01506] Monotonicity-preserving interpolation in multilevel schemes for balance laws
- [01433] Entropy-stable, positivity-preserving and well-balanced Godunov-type schemes for multidimensional shallow-water system
- [01511] Numerical solution of a system of conservation laws with discontinuous flux modelling flotation with sedimentation
- [01508] Implicit and IMEX Lagrange Projection schemes for Ripa model
- [01400] Vertical discretizations of Euler systems and application to bedload problems
- [01507] Numerical methods for viscoplastic flows : balancing precision and acceleration
- [01504] Digital Twins (DT) on geophysical extreme hazards. Using Tsunami-HySEA numerical model as DT for tsunami hazards.
- [01513] Novel schemes for overdetermined thermodynamically compatible hyperbolic systems

**[00533] Recovery and robustness of geometric fingerprints for point clouds and data**

- [04178] Recovering discrete Fourier spectra from random perturbations
- [04956] An information-theoretic perspective on the turnpike and beltway problems
- [04313] Curvature sets and curvature measures over persistence diagrams
- [05121] Learning with persistence diagrams
- [04676] Persistent cycle registration and topological bootstrap
- [05127] The Density Fingerprint of a Periodic Set and Persistent Homology
- [04866] Reconstruction of manifolds from point clouds and inverse problems

**[00534] Topological and geometric data analysis: theory and applications**

- [01514] Vietoris-Rips persistent homology, injective metric spaces, and the filling radius
- [01746] Reeb Order Method and its Application to Topological Flow Data Analysis
- [04575] Topological Node2vec: Graph Embeddings via Persistent Homology
- [04694] Data, Geometry, and homology
- [04865] Topological Representation Learning for Biomedical Image Analysis
- [05110] New Algorithms for Random Graph Embeddings
- [05318] Topological Deep Learning: Going Beyond Graph Data
- [01521] Topological approaches to higher-order interaction networks

**[00538] Mathematical modeling, analysis, and simulation for complex neural systems**

- [04042] Learning optimal models of statistical events in spontaneous neural activity
- [03841] The hierarchical organization of the Drosophila connectome
- [01437] The mechanism of abnormal beta-oscillation generated in striatum
- [03947] Maturation of neurons reconciles flexibility and stability of memory: dual structural plasticity in the olfactory system
- [01409] Mathematical mechanism underlying hierarchical timescales in the primate neocortex
- [04184] Computation with Adaptive Continuous Attractor Neural Networks
- [03884] Learning biological neuronal networks with artificial neural networks: Neural oscillations
- [01458] Reconstruction of Evolving Percepts in Binocular Rivalry Using Novel Model Network Dynamics

**[00539] Extreme value theory and statistical analysis**

- [03480] Asymptotic theory for extreme value generalized additive model
- [03597] Comparative study on accuracy of sample maximum distribution estimators in IID settings

- [02777] Subsampling inference for nonparametric extremal conditional quantiles
- [03093] Measuring non-exchangeable tail dependence using tail copulas

**[00545] Waves in complex and multiscale media**

- [03757] Effective waves in random particulate media: introduction and numerical validation
- [04234] Scattered wavefield in the stochastic homogenization regime
- [04262] Waves on Graphs
- [04615] Designing large-scale acoustic scattering systems using structural optimization and multiple scattering theory
- [04940] Bounds on the Quality-factor of Two-phase Quasi-static Metamaterial Resonators and Optimal Microstructure Designs
- [04245] Band structure and Dirac points of real-space quantum optics in periodic media
- [03889] Mathematics of in-gap interface modes in photonic/phononic structures in one dimension
- [04807] Recent advances in the theory of field patterns
- [05192] Water wave resonances between floating vessels: fundamentals to applications
- [03152] Broadband energy capture by an array of heaving buoys
- [04111] Graded arrays for spatial frequency separation and amplification of water waves

**[00550] Multi-scale analysis in random media and applications**

- [04699] Recent advances in quantitative stochastic homogenisation of nonlinear models
- [04559] Quantitative Homogenization for Nondivergence Form Equations
- [04584] Quantitative homogenization of elliptic system with periodic and high contrast coefficients
- [05476] On the lower spectrum of heterogeneous acoustic operators
- [03179] Boundary effects in radiative transfer of acoustic waves in a randomly-fluctuating medium delimited by boundaries
- [05197] Bloch analysis extended to weakly disordered periodic media
- [04385] Gamma-convergence and stochastic homogenisation for phase-transition models
- [05141] Anomalous diffusion of a passive tracer advected by the curl of the GFF in 2D
- [04734] Variance reduction methods in random homogenization by using surrogate models

**[00552] Homogenization theory and applications**

- [01750] On the rate of convergence in homogenization of time fractional Hamilton-Jacobi equations
- [01811] Discrete approximation of higher degree Laplacians
- [03559] Homogenization of the rate-independent evolution of a random heterogeneous, elasto-plastic spring network

**[00554] Pattern dynamics appearing in mathematical biology**

- [01234] Turing's instability by equal diffusion
- [01275] Reaction-diffusion fronts in funnel-shaped domains
- [01442] Traveling wave solution in a macroscopic traffic model
- [03160] Bistable pulsating fronts in showing oscillating environments

**[00555] Advanced Numerical Methods for PDEs with Applications**

- [02041] Numerical Methods for PDEs and Mesh Generation
- [01595] PDAEs redux
- [02132] Optimized Schwarz domain decomposition for surface intrinsic positive Helmholtz equations
- [02719] DD approaches for surface PDEs solved by the closest point method
- [02811] TVD property of second order method for two-dimensional scalar conservation laws
- [02206] Using Adaptive Time-Steppers to Explore Stability Domains
- [02320] Extended Statistical Modelling and Advanced Computational Approaches for Disperse Multiphase Flows
- [02260] tost.II: A temporal operator splitting template library for deal.II

**[00558] Bifurcations, periodicity and stability in fluid-structure interactions**

- [04678] Weak solutions in fluid-structure interactions: Cauchy and periodic problems
- [02192] Modelling and analysis of solids floating in a viscous fluid
- [02207] Time-periodic solutions to an interaction problem between a compressible fluid and a viscoelastic structure
- [02722] Artificial boundary conditions for time-periodic flow past a body
- [04833] On the motion of several small rigid bodies in a viscous incompressible fluid
- [05105] On the motion of a fluid-filled elastic solid
- [05124] Gevrey regularity of a certain fluid-structure PDE interaction
- [05184] Numerical benchmarking of FSI - efficient discretization and numerical solution

**[00559] DNB Theory and its Applications**

- [05641] DNB-based intervention for ultra-early treatment
- [05637] Alerting for the critical transition of complex systems
- [05638] The algorithm and application of landscape-DNB in complex disease of single sample
- [05640] DNB based network fluctuation and application to biology and medicine
- [05343] Change-point detection in temporal complex systems
- [05648] Early warning signals for multistage transitions in tipping dynamics on networks
- [03348] Modelling single cell multi-omics data

**[00563] PDE's on Mathematical Physics and Biology**

- [04143] The effect of diffusion on principal eigenvalues for Hamilton-Jacobi equations
- [03901] Population models with an interface region inside the domain
- [04005] A bifurcation result for a fractional semilinear Neumann problem
- [04254] Systems of coupled nonlinear Schrödinger equations
- [03153] Stable standing waves for a Schrödinger system with nonlinear chi^3 response

- [03664] Critical nonlocal problems driven by the fractional Laplacian
- [04405] Variational and topological methods on non-compact Randers spaces
- [00570] Title: Machine Learning and Statistical Approaches for PDE Based Inverse Problems in Imaging**
  - [04498] Train Like a (Var)Pro: Efficient Training of DNNs
  - [05369] Machine Learning for Inverse Problems in Electrical Impedance Tomography
  - [04986] Data-Driven Design of Thin-Film Optical Systems using Deep Active Learning
  - [04138] Implicit Solutions of Electrical Impedance Tomography Using Deep Neural Network
- [00571] Mathematics in biological pattern formation: modeling, analysis, and applications**
  - [04548] Patterning conditions in bilayer reaction-cross-diffusion systems
  - [04979] Multilevel mathematical modeling methods for morphogenesis of bacterial cell populations
  - [04657] A continuous model for bacteria growth with short range interactions, growth and interaction: derivation and analysis of pattern formation
  - [03139] Approximation for nonlocal Fokker-Planck equations by a Keller-Segel system
- [00573] Emerging Methods for Shape- and Topology Optimization**
  - [02707] Geometry Segmentation with Total Variation Regularization
  - [03021] Topology optimisation with general dilatations via the topological state derivative
  - [03573] Combining parameterized aerodynamic shape optimization with Sobolev smoothing
  - [03630] A combined phase field - Lipschitz method for PDE constrained shape optimization
  - [04267] Interface Identification constrained by Local-to-Nonlocal Coupling
  - [04673] Total Generalized Variation for Geometric Inverse Problems
  - [04738] Choice of Inner Product in Shape Gradient Descent
  - [04786] Image and Shape Registration via Transport Equations
- [00574] Recent Progress on Stochastic Analysis, Control, and their Applications**
  - [03197] Continuous-Review Inventory Systems with Discontinuous Setup Costs
  - [04097] Deep learning methods in insurance and risk management
  - [04139] Exponential stability of stochastic functional differential equations with impulsive perturbations
  - [03618] Fully-coupled two-time-scale stochastic functional differential equations with infinite delay
  - [03662] On the weak stability and stabilization of McKean-Vlasov stochastic differential equations
  - [05067] Limit Theorems for Distribution Dependent Jump Processes with Random Switching
  - [03342] From the optimal singular stochastic control to the optimal stopping for regime-switching processes
- [00575] Factors and Cycles**
  - [02338] On cycles and factors in graphs with large degree sum
  - [02275] Toughness and forbidden subgraphs for graphs to be hamiltonian
  - [02216] Recent progress on distance matching extension in graphs on surfaces
  - [02696] Eigenvalues and factors in regular graphs
- [00580] Mathematical Challenges in Current and Future Location Estimation Systems**
  - [01325] Local Strong Convexity of Source Localization and Error Bound for Target Tracking under Time-of-Arrival Measurements
  - [01604] Machine learning techniques for resolving GNSS integer ambiguities
  - [01656] Fast and almost unbiased position estimation for location service
  - [01296] Robust Location Estimation in Wildlife Tracking Systems
- [00581] Analysis, Methods and Applications in Complex Materials**
  - [04090] A framework for a generalization analysis of MLIPs
  - [04086] A Finite Element Configuration Interaction Method for Wigner Localization
  - [05440] Equivariant Tensor Network Potentials
  - [04136] Planewave approximation for electronic structure calculation of incommensurate systems
  - [04088] DeePN2: A Deep Learning-Based Non-Newtonian Hydrodynamic Model
  - [04357] Numerical Analysis of Structural Green's Function in Multiple Scattering Theory
  - [04087] Variational Monte Carlo from a Continuous Viewpoint
- [00584] Advanced Methods for Structured Eigenvalue Problems and Nonlinear Equations**
  - [01505] Eigen-decomposition and Fast Solvers for Maxwell's Equations for 3D Photonic Crystals
  - [01246] Projected Gradient Method for Volume-Measure-Preserving Optimal Mass Transportation Problems
  - [01095] Multitask kernel-learning Gaussian process regression parameter prediction method and its application in matrix splitting iteration methods
  - [01322] Breakdown Avoidance Structure-Preserving Doubling Algorithms for Nonlinear Matrix Equations
  - [01293] Newton-Noda iteration for nonlinear eigenvalue problems
  - [01584] Phase Retrieval of Quaternion Signal via Wirtinger Flow
  - [01454] Numerical Methods for the Complete Solution of Multiparameter Eigenvalue Problems
  - [02763] Perturbation theory for the symmetry eigenvalue problem and singular value decomposition followed by deflation techniques
  - [01112] Nonlinear Energy Minimization for Simplicial Manifold Parameterizations
  - [01534] Two harmonic Jacobi-Davidson methods for computing a partial GSVD of a large matrix pair
  - [01473] Harmonic multi-symplectic Lanczos algorithm for quaternion singular triplets
  - [01319] The asymptotic analysis of generalized orthogonal flows
- [00586] Challenges for Attaining High-performance in Numerical Software**
  - [03413] Adaptation of XAI to Numerical Libraries: A Case Study for Automatic Performance Tuning

- [03472] Parallel Eigensolvers Based on Minimization Strategies
- [03700] Mixed-precision iterative refinement for real-symmetric eigenvalue decomposition with clustered eigenvalues
- [04170] Mixed Precision Iterative Refinement with H-matrices

**[00587] Recent Advances in Numerical Methods for Nonlinear Hyperbolic PDEs**

- [01485] A New Locally Divergence-Free Path-Conservative Central-Upwind Scheme for Ideal and Shallow Water Magnetohydrodynamics
- [01517] Geometric Quasilinearization (GQL) for Bound-Preserving Schemes of Hyperbolic PDEs
- [01722] An improved non-hydrostatic shallow-water type model for the simulation of landslide generated tsunamis
- [01949] A New Approach for Designing Well-Balanced Schemes for the Shallow Water Equations
- [02636] Error analysis of finite volume methods for the Euler equations via relative energy
- [04782] Flux Globalization Based Well-Balanced Path-Conservative Central-Upwind Schemes
- [01953] High order well-balanced and asymptotic preserving WENO schemes for the shallow water equations

**[00589] Computational Biomedical Physics and Mechanics**

- [01471] A Multi-Scale Approach to Model K+ Permeation Through the KcsA Channel
- [02551] Modeling electrohydrodynamic flow through a nanochannel
- [02740] Double diffusion for nanofluid
- [03003] GPU Computation of High-Intensity Focused Ultrasound Ablation Under Different Pathways

**[00592] Optimization and Inverse Problems**

- [03137] Sparsity-promoting regularization for inverse problems via statistical learning
- [03391] Online Optimization for Dynamic Electrical Impedance Tomography
- [03177] Primal-Dual Methods with Adjoint Mismatch
- [02036] Material decomposition in multi-energy X-Ray tomography with Inner Product Regularizer
- [05012] Multiscale hierarchical decomposition methods for ill-posed problems
- [05199] Multiscale hierarchical decomposition methods for images corrupted by multiplicative noise
- [03502] A Lifted Bregman Formulation for the Inversion of Deep Neural Networks
- [03398] Stable Phase retrieval with mirror descent

**[00593] Advances in Nonlinear Dynamics**

- [02779] Polynomial discretisations of transfer and Koopman operators in chaotic dynamics
- [03719] Estimating the spectra for annealed transfer operators of random dynamical systems
- [03734] Energy growth in Hamiltonian systems with small dissipation
- [03874] A dynamical systems approach to low-damage seismic design
- [03886] Understanding how blenders emerge: weaving a carpet from global manifolds
- [03948] A Dynamical Systems Approach for Most Probable Escape Paths over Periodic Boundaries
- [04096] On the connectedness and disconnectedness of the Julia set for the Hénon map.
- [04135] Standard piecewise smooth symplectic maps
- [04300] Optimal linear response for expanding circle maps
- [04937] Finite element approximated manifolds for PDEs by the parameterization method
- [05240] Dynamics of a Hill four-body problem with oblate bodies
- [05259] Parametrisation method for large finite element models of engineering structures

**[00595] Combinatorial topological dynamics**

- [05133] Analyzing Network Representations of Dynamical Systems Using Persistent Homology
- [01382] Topological Data Analysis of Spatiotemporal Honeybee Aggregation
- [03128] What does Multivector Fields Theory have to offer?
- [03410] A Persistence-like Algorithm for Computing Connection Matrices Efficiently
- [04935] A combinatorial/homological framework for continuous nonlinear dynamics
- [04988] Computing the Global Dynamics of Parameterized Systems of ODEs
- [04981] Combinatorics and Topology for Understanding Global Dynamics in Multi-Scale Systems.
- [04843] On the identification of cycling motion using topological tools
- [03335] Morse-Smale quadrangulations and persistence of vector fields
- [04607] On the dynamics of the combinatorial model of the real line
- [04886] Topological Inference of the Conley Index
- [05010] Analysis of solids regarded as compositions of discrete entities

**[00598] Hyperplane arrangements and enumerative problems**

- [01887] Coboundary polynomial and related polynomial invariants
- [01889] Generalizations of Tutte-Grothendieck polynomials
- [01791] Characteristic quasi-polynomials of arrangements over algebraic integers
- [01780] Counting the regions of hyperplane arrangements related to Coxeter arrangements.

**[00603] Mean field stochastic control problems and related topics**

- [01320] Stochastic maximum principle for weighted mean-field system
- [00653] The mass-conserving stochastic partial differential equation coming from spatial mean-field term
- [01321] A quadratic mean-field BSDE with its applications
- [01324] Mean field stochastic control under sublinear expectation

**[00604] Frontiers of Collaboration with Industry: Towards International Mathematical Commons**

- [01978] The UniSA Mathematics Clinic: How to build a work-integrated-learning ecosystem
- [02932] Industrial Student Research Programs and Industry Connections at IPAM
- [01963] Development of Mathematics for Industry in Japan: New Research Area, Education and Platform

- [01984] APCMFI and International Mathematical Commons for Asia Pacific region
- [01944] European Consortium for Mathematics in Industry - research and education
- [01965] EU-MATHS-IN OpenDesk. Un infrastructure to boost industry's competitiveness.
- [02986] mathematics in the society: rethinking its role, one graduate student at a time.
- [05594] A Knowledge Exchange Hub for the Mathematical Sciences

**[00605] Recent advances in theory and application of quantum computing technology**

- [03620] QUBO encoding of inequality constraints in Quantum Minimum Fill-in algorithm
- [02807] Approximate block diagonalization of symmetric matrices using a quantum annealing
- [03304] Performance evaluation of quantum-inspired machine and quantum simulator
- [03892] Use of digital annealer for HPC applications
- [04414] Performance Evaluation of Ising Machines using Constraint Combinatorial Optimization Problems
- [04218] Nonnegative binary matrix factorization by continuous relaxation and reverse annealing
- [03976] Kernel learning by quantum annealer
- [03609] mpiQulacs: A Distributed Quantum Computer Simulator for A64FX-based Cluster Systems
- [04257] Examples of application of CMOS annealing
- [04116] Outline and present development status of CMOS annealing

**[00607] Analysis and computation of interface evolution equation and related topics**

- [03814] A minimizing movement approach to surface constrained interfacial motions
- [02801] Geometric Sobolev gradient flows on spaces of curves
- [03938] A Simple Algorithm for the Monge-Ampere Equation on a Sphere
- [02029] Waiting time effects for the wearing process of a non-convex stone

**[00608] Limit behavior and asymptotic properties in fluid mechanics**

- [01787] Homogenization of nonstationary incompressible viscous non-Newtonian flows
- [05572] Homogenization of compressible Navier-Stokes in critically perforated domains in Limit behavior and asymptotic properties in fluid mechanics
- [05422] Existence of weak solutions and hard-congestion limit in the dissipative Aw-Rascle system
- [01575]  $\Gamma$ -convergence of nearly incompressible fluids
- [04842] Invariant manifolds for the thin film equation
- [03881] The Navier-Stokes flow in the exterior Lipschitz domain
- [04533] Anisotropically spatial-temporal behavior of the Navier-Stokes flow past an obstacle
- [01603] Stokes and Oseen fundamental solutions: asymptotic properties of fluid flows and applications in computational fluid dynamics
- [04660] Multiscale analysis - from compressible to incompressible system
- [04114] Mixing and enhanced dissipation for fluid suspensions
- [05036] Resolvent estimate for the Stokes equations in the Besov spaces
- [05215] Conditions for energy balance in 2D incompressible ideal fluid flow

**[00612] New models and methods for capacity planning and scheduling**

- [01483] Joint replenishment combined with machine scheduling: offline and online algorithms
- [01552] Sequential testing in batches with resource constraints
- [00764] A flow-based formulation for parallel machine scheduling using decision diagrams
- [00808] Parallel Machine Scheduling Under Uncertainty: Models and Exact Algorithms
- [02307] Energy-aware flow shop scheduling with uncertain renewable energy
- [02657] An effective model-driven heuristic algorithm for the collaborative operating room scheduling problem
- [01493] Valid inequalities for the parallel stack loading problem of minimizing the number of badly-placed items
- [01466] Branch-and-Price-and-Cut for the Team Orientation Problem with Interval-Time-Varying Profit
- [03681] A hybrid algorithm of integrated container truck scheduling problem
- [05024] Compact formulations for parallel machine scheduling with conflicts
- [01311] Project scheduling under various resource constraints

**[00615] Nonlinear PDEs & Probability**

- [04215] A mixed-norm estimate of two-particle reduced density matrix of many-body Schrödinger dynamics for deriving Vlasov equation
- [03911] Hydrodynamic limit equations derived from microscopic interacting particle systems
- [01645] The Vicsek-BGK equation in collective dynamics
- [03240] Quasilinear SPDEs with rough paths
- [03798] A regularity structure for the quasilinear generalized KPZ equation
- [03415] Gradient continuity of weak solutions for perturbed one-Laplace problems
- [02739] Asymptotic behavior of geometric flows with contact angle conditions
- [05334] Weak-strong uniqueness for volume-preserving mean curvature flow

**[00616] Continuous optimization: theoretical and algorithmic trends**

- [03840] Constant rank constraint qualification for nonlinear second-order cone programming
- [03851] Strong global convergence properties of an Augmented Lagrangian method for symmetric cones
- [02990] On enhanced KKT optimality conditions for smooth nonlinear optimization
- [03586] Adaptive Third-Order Methods for Composite Convex Optimization
- [03706] On the globalization of nonlinear programming methods.
- [04137] Proportionality based algorithms for quadratic programming
- [03943] On the Inexact Restoration approach for adaptive sample size in finite sum minimization

[03290] Block coordinate descent and the close enough traveling salesman problem

[02948] Sequential optimality conditions: how to stop optimization algorithms

[01945] Distributed Inexact Newton Method with Adaptive Step Sizes

**[00621] Frontiers of Collaboration with Industry: Succeeding through Failure**

[01441] Mobility Optimization Engine and its Real-world Applications

[02078] Mathematical modeling with industry in the water sector: what makes good practice

[01474] An international research program on industrial problems for math students.

[02098] Collaboration with early graduate researchers, and improvements on simulated annealing

[02914] Development of a CNN-Based Model for Car Classification and Damage Detection from car accidents

[03805] Failure and Success for Bauxite Moisture Measurement with Microwaves

[02161] The UniSA Mathematics Clinic: Renewables, defence, mining, drones, and justice

[01470] Interdisciplinary research using Topological Flow Data Analysis through Math Clinic

**[00622] Inverse Problems and Imaging**

[01259] Testing statistical hypothesis in Inverse Problems

[01346] Disentangling domain bias in medical images for meaningful embeddings

[01553] A Bregman-Kaczmarz method for nonlinear systems of equations

[01556] A complementary  $\ell^1$ -TV reconstruction algorithm for limited data CT

[01577] 3D image reconstruction for cone beam computed tomography using sparsity

[01591] High Dynamic Range Tomography via Modulo Radon Transform

[01593] A new inversion scheme for elastic diffraction tomography

[01606] inverse electromagnetic scattering problems with internal dipoles

[03917] A paraxial approach for the inverse problem of vibroacoustic imaging

[05513] Primal-dual proximal splitting and generalized conjugation in non-smooth non-convex optimization

**[00624] At the interface between neural networks and differential equations**

[01481] Operator learning and nonlinear model reduction by deep neural networks

[01838] A deep learning framework for geodesics under spherical Wasserstein-Fisher-Rao metric

[01927] Mean-field Analysis of Piecewise Linear Solutions for Wide ReLU Networks

[02274] On the Mean-field Theory of Neural Network Training

[01535] Machine learning for/with Differential Equation Modeling: Statistics and Computation

[02223] Momentum Based Acceleration for Stochastic Gradient Descent

[03468] The Effects of Activation Functions on the Over-smoothing of GCNs

[03523] On the generalization and training of Deep Operator Networks

**[00625] Mathematical Modeling and Combinatorial Optimization**

[02230] Sports Scheduling: Number of Trips in the Traveling Tournament Problem

[04421] Efficient allocation of demand to facilities on road networks

[01600] Optimal UAV Flight Path Planning for Herding Sheep

[02992] Formulations and algorithms for a square independent packing problem

[02859] A core selection method for the robust traveling salesman problem

[02909] Algorithms for two-machine job-shop scheduling problem with one joint job

[04538] A New Multivariate Decision Tree Based on Mixed Integer Linear Programming

[04561] A Linear Delay Algorithm for Enumeration of 2-Edge/Vertex-connected Induced Subgraphs

**[00626] Finite element complexes for structure-preservation in continuum mechanics**

[02976] Finite element gradgrad and divdiv complexes in three dimensions

[05087] Structure-preserving discretization for wave equations

[03866] Regge finite elements and the linearized Einstein tensor

[03058] Variational structures in cochain projection based discretization of classical field theories

[02047] Local Exactness of de Rham Conforming Hierarchical B-spline Differential Forms

[02065] Multigrid solvers for the de Rham complex with optimal complexity in polynomial degree

[04622] On partially continuous finite element spaces in variational problems of continuum mechanics

[05396] New Class of Stabilized Mixed FEM for Compressible and Incompressible Nonlinear Elasticity

[05491] Machine-Learned Whitney Forms for Structure Preservation

[04438] Study of a structure preserving discretization framework for Maxwell-Klein-Gordon equations.

[05131] Compatible finite elements for terrain following meshes

[04775] Structure-preserving discretization of momentum-based formulations of fluids using discrete exterior calculus

**[00632] From model-blind to model-aware learning of inverse problems in imaging**

[03849] Untrained networks with latent-space disentanglement for motion separation in videos

[01569] Continuous Generative Neural Networks for Inverse Problems

[02780] Learned proximal operators in accelerated unfolded methods with pseudodifferential operators

[02946] Electrical impedance tomography, virtual X-rays, and stroke

[03308] Beyond supervised learning in imaging: measurement-driven computational imaging

[03519] Deep Learning for Reconstruction in Nano CT

[04062] Learning intrinsic shape representations via LBO spectra

[04272] Inexact Algorithms for Bilevel Learning

**[00633] Unconventional numerical methods for advection-diffusion PDEs**

[03915] Dissipation-based WENO stabilization of high-order finite element methods for hyperbolic problems

[04012] A Residual Distribution Approach to Isotropic Wave Kinetic Equations

- [04019] High order Flux Reconstruction schemes for turbulent flows and spectral analysis
- [04429] The Cartesian Grid Active Flux Method with Adaptive Mesh Refinement
- [04883] Optimization-based, property-preserving algorithm for passive tracer transport
- [04980] Multi-material ALE remap: interface sharpening in a matrix-free computation
- [05104] Robust second-order approximation of the compressible Euler Equations with an arbitrary equation of state
- [05153] Heuristic Topological Estimation of Reduced Order Model Basis Functions from PDE Solution Snapshots
- [00635] Mean field games and optimal transport with applications in data science and biology**
  - [05205] Manifold Interpolating Optimal-Transport Flows for Trajectory Inference
  - [01462] A Distributed Algorithm for Wasserstein Proximal Operator Splitting
  - [05216] Wasserstein gradient flows and Hamiltonian flows on the generative model
  - [05393] Linear Optimal Transport (LOT) Framework for Graph-Based Semi-Supervised Learning using Point Cloud Data
  - [05294] Towards a mathematical theory of development
  - [03712] Applications of Gromov-Wasserstein Distance to Graph and Hypergraph Analysis
  - [03382] Single-cell data integration using optimal transport
  - [03962] Multi-agent reinforcement learning for collaborative games: a mean-field perspective
- [00638] Minisymposium on Interaction between Harmonic Analysis and Data Science**
  - [01801] Algorithms for quantizing neural networks with guaranteed accuracy
  - [01538] Learning nonlinear functionals using deep ReLU networks
  - [01578] Compressed sensing for the sparse Radon transform
  - [01808] Super-resolution of sparse measures: recent advances
  - [04107] Proximal neural networks and Plug-and-Play methods
  - [03587] The Bayesian Learning Rule
  - [02888] Learning linear operators: Infinite-dimensional regression as a well-behaved non-compact inverse problem
  - [02915] A Non-Asymptotic Analysis of Dropout in the Linear Model
  - [04309] Direct method for function approximation on data defined manifolds, II
  - [04364] Distribution learning for count data
  - [05188] Hierarchical systems of exponential bases for partitions of intervals
- [00639] Analytical and computational aspects of topological photonics**
  - [03761] TE band structure of high contrast honeycomb photonic crystals
  - [03902] Super band gaps and interface modes in one-dimensional quasicrystals
  - [03872] Mathematical theory for the interface mode in a waveguide bifurcated from a Dirac point
  - [05154] Bloch Waves for Maxwell's Equations in High-Contrast Photonic Crystals
  - [05207] Pseudo-magnetism and Landau Levels in strained 2-dimensional photonic crystals
  - [05298] Quantized Fractional Thouless Pumping of Solitons
  - [04812] Topological insulators in semiclassical regime
  - [05311] Topological-cavity surface-emitting laser
- [00640] Variational Analysis: Theory and Applications**
  - [01802] Fixed point strategies for sparsity aware inverse problems and hierarchical convex optimization
  - [02724] The splitting algorithms by Ryu, by Malitsky-Tam, and by Campoy applied to normal cones of linear subspaces converge strongly to the projection onto the intersection
  - [02977] Fixed Point Algorithms: Convergence, stability and data dependence results
  - [01896] Adaptive proximal algorithms for convex optimization under local Lipschitz continuity of the gradient
  - [02427] Level proximal subdifferential and its resolvent
  - [02993] On quasidifferentiability and optimization problems
- [00641] Emerging Collaborations: Mathematical Views of Modelling Biological Scales**
  - [01865] A Multiscale, Interdisciplinary Approach to Blood Clot Degradation
  - [01970] Explorations of DNA Knot Shadows
  - [02104] A mathematical approach to understanding reproductive health disparities at the intersection of ovulatory and metabolic dysfunction
  - [02133] Harmonic Analysis on Simplicial Simplexes: How far could we take it?
  - [02145] Ecological consequences of heterogeneity in host-pathogen population dynamics
  - [02146] Modeling microscale biofluids
  - [02152] We are what we eat: a mathematical model of the gut-brain axis.
  - [02213] Modeling the long term effects of thermoregulation on human sleep
- [00642] Traveling Waves in Mathematical Epidemiology**
  - [05106] Traveling wave solutions for an epidemic model with free boundary
  - [01447] Traveling Wave Solutions for Discrete Diffusive SIR Epidemic Model
  - [04496] Traveling waves of a differential-difference diffusive Kermack-McKendrick epidemic model with age-structured protection phase
- [00643] Stochastic modeling in cell biology**
  - [04558] Intracellular Transport Across Scales
  - [02757] Inferring RNA Dynamic Rates from Spatial Stochastic Snapshots
  - [02952] Centrosome Movement and Clustering During Mitosis
  - [01821] Stochastic model of nuclear size control in *S. pombe*
  - [05399] Stochastic models of DNA methylation, plasticity and drug resistance
  - [04460] Stochastic modeling of ovarian aging

- [02211] Optimal curvature and directional sensing in long-range cell-cell communication
- [04467] Centrosome asymmetry in the early *C. elegans* embryo
- [04462] Modeling and tracking random motion in micrometer-scale living systems
- [04071] Stochastic effects in molecular motor teams under detachment and reattachment

**[00652] Recent Advances in Quasi-Monte Carlo Methods and Related Topics**

- [04989] The fast reduced QMC matrix-vector product
- [05066] Recent Advances on discrepancy and WCE of constructible point sets on spheres
- [03448] Quasi-Monte Carlo approach to Bayesian optimal experimental design
- [04877] Density estimation by Monte Carlo and quasi-Monte Carlo
- [03343] High dimensional approximation and the curse of dimensionality
- [01697] QMC and sparse grids beyond uniform distributions on cubes
- [02052] Can hyperinterpolation part with quadrature exactness?
- [04553] Quasi-Monte Carlo-Based Algorithms for Deep Learning with Applications
- [04614] Lattice rules for integration on  $\mathbb{R}^d$
- [04320] SNPE-B Revisited: Rethinking of Data Efficiency and Variance Reduction
- [04916] Variable importance measures in high dimensional data sets
- [03703] Tuning QMC point sets using WAFOM-like value

**[00654] Poset Combinatorics**

- [02151] The operad of finite posets acts on zeta values
- [01777] What is -Q for a poset Q?
- [04172] A new expression for the order polynomial
- [02099] Polychrony as chinampas

**[00656] Multiscale Pattern Formation**

- [01951] Multiscale pattern formation in space and time
- [01983] Localized spot dynamics: curvature and instability
- [01901] Spiky patterns in a three-component consumer chain model
- [01941] Emergence of locomotion by autonomous parameter tuning
- [01917] Symmetry-Breaking for a Compartmental-Reaction Diffusion System
- [01765] Bayesian Model Selection of PDEs for Pattern Formation
- [02979] Spectral Stability of Far-from-Equilibrium Planar Periodic Patterns
- [01867] Fronts in the wake of a slow parameter ramp
- [02507] Front propagation in a multi-variable morphogenetic model of branching
- [02105] CONTROL OF ENGULFMENT FOR BINARY POLYMER PARTICLES
- [03494] Instability of Planar Interfaces in Reaction-Diffusion-Advection Equations
- [04510] Patterns on patterns

**[00657] Tomographic inverse problems and deep learning techniques**

- [05264] Ill-posed Inverse problems in Low-dose Dental Cone-beam Computed Tomography
- [05265] Machine learning for automatic signal quality assessment in multi-channel electrical impedance-based hemodynamic monitoring
- [05332] Application of AI-based Medical Diagnosis: focusing on tomography
- [05324] Data-driven reconstruction in X-ray CT with provable convergence guarantees

**[00666] Simulations and Algorithms for Materials Sciences**

- [02135] ESES, a Eulerian and Lagrangian molecular surface generator
- [02756] From nanocrystals to glasses: a strengthening mechanism analysis for amorphization.
- [02794] Sum-of-Gaussians method with applications to molecular dynamics simulations
- [03201] Random-batch Ewald method for molecular dynamics
- [04335] Molecular Dynamics Simulation of Concentrated Entangled Polymers in Athermal Solvents
- [04386] Multiscale modeling and Simulations of Interfacial Defects in based on PN model
- [04817] Solving integral equations on non-smooth boundaries
- [05284] A fast algorithm for Dirichlet partition problems

**[00669] Mathematical Solutions of Industrial Applications**

- [02716] Prediction of Leaf Area Index of Tomato Plants by Image Processing and Deep Learning
- [02893] Frequency based graph estimation for multivariate time-series
- [02900] Passive Gamma Emission Tomography for Spent Nuclear Fuel
- [02901] Boundary estimation of the X-ray tomographic reconstruction using persistent homology

**[00670] Financial Risk Management and Related Topics**

- [03276] Discrepancy between Regulations and Practice in Initial Margin Calculation
- [02781] Last Passage Time and its Applications in Risk Management
- [04631] Construction and sample path properties of Brownian house-moving
- [02599] Stability of High Order Moments: a Risk Management Approach
- [03952] Gross-revenue-based structural credit risk model
- [03406] Insider vs. Outsider: Information and Enlargement of Filtrations
- [02711] Sparse factor model of high dimension
- [03676] On a measure of tail asymmetry for the bivariate skew-normal copula

**[00672] Efficient inference for large and high-frequency data**

- [05600] Fast and asymptotically efficient inference for large and high-frequency data

- [05624] On Adaptive Kalman Filtration
- [05359] Fast calibration of weak FARIMA models
- [05613] Fast Inference for Stationary Time Series
- [03747] Local asymptotic property for the Euler approximation of SDE driven by a stable Lévy process
- [03713] Asymptotics for Student-Lévy regression
- [01903] High-frequency estimation of pure jump alpha-CIR process
- [02309] Local asymptotic properties for the growth rate of a jump-type CIR process
- [01940] Statistical inference for rough volatility: minimax theory
- [01388] Statistical inference for rough volatility: Central limit theorems
- [02004] A GMM approach to estimate the roughness of stochastic volatility
- [01999] Asymptotically Efficient Estimation for Fractional Brownian Motion with Additive Noise
- [00673] Recent advances in discontinuous Galerkin methods and the related applications**
  - [03246] Bound preserving DG methods for multi-species flow with chemical reactions
  - [03960] Staggered discontinuous Galerkin methods for the Stokes problem on rectangular grids
  - [02857] A mass conservative scheme for the coupled flow and transport
  - [03078] hp-Multigrid preconditioner for a divergence-conforming HDG scheme for the incompressible flow problems
  - [04124] Numerical Modelling of the Brain Poromechanics by High-Order Discontinuous Galerkin Methods
  - [03151] Cell-average based Neural Network method for time dependent PDEs
  - [04606] A non-overlapping Schwarz algorithm for the HDG method
  - [03898] Adaptive methods for fully nonlinear PDE
- [00674] Modern numerical methods for PDE-constrained optimization and control**
  - [03637] Recent Developments in Preconditioning for PDE-Constrained Optimization
  - [01670] GKBO method for global optimization of non-convex high dimensional functions.
  - [01649] Online identification and control of PDEs via RL methods
  - [03371] A statistical POD approach for feedback boundary optimal control in fluid dynamics
  - [04310] Optimal Control of Some Nonlocal PDEs
  - [01642] Decentralized strategies for coupled shape and parameter inverse problems
  - [04057] Stability-exploiting adaptive finite elements for optimal control
- [00675] New trends in (optimal) control theory**
  - [01796] Surveillance-evasion games with visibility constraints
  - [01823] Steering undulatory micro-swimmers in a fluid flow through reinforcement learning
  - [02637] Optimization problems under uncertainty
  - [01828] Stability of open quantum systems designed by reservoir engineering.
  - [01818] Turnpike phenomena in optimal control
  - [02571] Stabilization of traffic flow using fixed bottlenecks
  - [02530] Optimal Boundary Control for the semilinear Transport Equation under Uncertainty: A Turnpike Result
- [00685] Mathematical modeling, simulation and optimization in stroke risk assessment**
  - [03136] Hemodynamic modeling of directional shear risk metrics in the carotid artery
  - [03760] Physiological flow simulations for stroke assesment and importance of distensiblity
  - [03568] Predicting Stroke Risk with Graph Neural Networks and CFD Simulations
  - [03834] Shape optimization in applications of blood flows under uncertainties
- [00686] Higher-order networks for complex systems**
  - [02953] Towards mixed volumes of binomial reaction networks
  - [02968] A Hypergraph Model of Opinion Dynamics
  - [02963] Topological techniques for classification of agent-based tumour-immune model
  - [02931] Topological methods for spatial data in molecular biology
  - [02955] Clustering and trajectory classification via the Hodge Laplacian
  - [02956] Kernel-based independence measures, hypergraphs, and higher-order interactions
  - [02966] Higher-Order Phase Oscillator Networks from Phase Reductions
  - [03193] When do two networks have the same steady state ideal?
  - [02960] Hypergraph representation of topological features in complex systems
  - [02964] Spectral theory of graphs and hypergraphs
  - [02989] Role analysis for higher-order social systems
  - [02951] Topological Information Retrieval with Dilation-Invariant Bottleneck Comparative Measures
- [00687] Recent advances in deep learning-based inverse and imaging problems**
  - [05273] Data-driven parameter optimization for some inverse problems with sparsity-based priors
  - [03185] Data-driven Joint Inversion for PDE Models
  - [02972] A scalable deep learning approach for solving high-dimensional dynamic optimal transport
  - [04688] Learning nonlinearities in time-dependent PDEs from data
  - [04070] Conductivity imaging using deep neural networks
  - [04396] Model-corrected learned primal-dual models for fast photoacoustic tomography
  - [03165] Learning the Regularisation Parameter for Inverse Problems
  - [04247] Lipschitz Training for Adversarially Robust Neural Networks
  - [05448] The Unrolled Dynamics Modeling for Computed Tomography
  - [04836] Dictionary learning for an inverse problem in quantitative MRI
  - [05295] Deformable volumetric Image registration based on unsupervised learning

**[00690] Computational methods for interfaces in physics and mechanics**

- [01367] Computation of free boundary minimal surfaces via extremal Steklov eigenvalue problems
- [05329] Capturing surfaces using differential forms
- [05617] Nonlocal approximations of anisotropic surface energies on partitions
- [05463] On some extensions and applications of thresholding schemes
- [05615] Advanced discretization schemes for phase-field fracture
- [01899] Numerical approximation of a viscoelastic Cahn–Hilliard model for tumour growth
- [02809] A second order Cahn–Hilliard model for wetting simulation
- [04707] Finite element minimization of line and surface energies arising in liquid crystals

**[00696] Scientific Machine Learning for Inverse Problems**

- [03211] Learning Stochastic Closures Using Sparsity-Promoting Ensemble Kalman Inversion
- [03315] Efficient Bayesian Physics Informed Neural Networks for Inverse Problems via Ensemble Kalman Inversion
- [02563] Neural operator acceleration of PDE-constrained Bayesian inverse problems: Error estimation and correction
- [01533] Ensemble Kalman inversion with dropout in Scientific Machine Learning for Inverse Problems
- [03213] Projected variational inference for high-dimensional Bayesian inverse problems
- [03215] Multifidelity deep neural operators for efficient learning of partial differential equations with application to fast inverse design of nanoscale heat transport
- [02629] Surrogate modeling for many-body hydrodynamic interactions via graph neural networks
- [04531] A practical use of neural density estimators for Bayesian experimental design
- [03214] Solving High-dimensional Inverse Problems with Weak Adversarial Networks
- [01482] Automatic discovery of low-dimensional dynamics underpinning time-dependent PDEs for inverse problems resolution

**[00699] Delay and stochastic differential equations in life sciences and engineering**

- [04596] Impacts of demographic and environmental stochasticity on population dynamics with cooperative effects
- [03954] Recent advances in modeling tick-borne dynamics using delay differential equations
- [03402] Delay and Resonance: From Differential Equations to Random Walks
- [03310] Evolutionary Games with Strategy-Dependent Time Delays
- [03461] Asymptotic behaviour for nonautonomous Nicholson equations with mixed monotonicities
- [03291] Periodicity and stability in some biological delay models
- [03816] Exponential stability of linear discrete systems with multiple delays
- [03498] On asymptotic stability of equations and systems with distributed, unbounded and infinite delays
- [04635] Asymptotic classification of forced stochastic systems with memory
- [04851] Asymptotic analysis of stochastic functional differential equations
- [03977] An order-one adaptive scheme for the strong approximation of stochastic systems with jumps.
- [02373] Mathematical Model of Hepatitis B Virus Combination Treatment
- [04297] The Impact of Time Delays on Synchrony in a Neural Field Model
- [03295] Stability analysis of coupled feedback in hematopoiesis

**[00702] Sequential Decision Making for Optimization, Learning and Search**

- [04910] Combinatorial 3D Shape Assembly with Sequential Decision-Making Processes
- [05274] Constraint active search as an alternative to optimization
- [05604] Optuna: A Software to Solve Black-box Optimization
- [05288] Evolution Strategies: Principles and Practical Issues

**[00703] Combining machine learning with domain decomposition and multilevel methods**

- [03764] A Domain Decomposition-Based CNN-DNN Architecture for Model Parallel Training
- [03312] DNN-MG: A Hybrid Neural Network/Finite Element Method
- [05268] Combining physics-informed neural networks with multilevel domain decomposition
- [04823] Enhancing training of scientific machine learning applications
- [04378] A Splitting Approach of Multilevel Optimization with an Application to Physics Informed Neural Networks
- [04367] Improved Accuracy of Physics-Informed Neural Networks Using a Two-Level Training Approach and Lagrange Multipliers

**[00704] Numerical Software Libraries Enabling Benefits to Scientific Applications**

- [01829] The Need of Ecosystems of Numerical Libraries for Applications
- [01773] Factorization based sparse solvers and preconditioners for robust solutions
- [01874] Exploring the HPC Frontier with Ginkgo
- [01866] Scalability Study for Planewave DFT Solvers
- [01830] Overview and Application Experiences with SUNDIALS
- [01626] Experience with Exascale Applications using PETSc/TAO
- [01703] On the Design and Performance of Exascale Applications using the Trilinos Solver Framework
- [01837] Paving the road for efficient volume coupling with preCICE
- [01915] MFEM: Accelerating Efficient Solution of PDEs at Exascale
- [01650] Exascale-Ready Adaptive Mesh Refinement Applications with AMReX
- [01911] Supporting Applications with the Chombo Framework
- [01456] Firedrake: Math to Supercomputer

**[00707] Theoretical and Numerical Challenges in the Modelling of Fluid Motion**

- [03903] Paradigm and Long-Time Evolution of Localized Solutions of Wave Systems: Consistency vs Integrability
- [05180] Modelling of tsunami generated by submarine volcanic eruptions in stratified oceans.

[05211] Physics-informed neural network for computating steady periodic water waves

[01814] Pressure distribution on seawalls due to wave effects

[02962] Internal waves, Coriolis force and undercurrents

[05173] On three dimensional models of equatorial ocean flows

[03835] Eddy viscosities and ageostrophic wind-speed profiles

#### **[00708] Computational medicine of the heart: towards cardiac digital twins**

[04495] Multiphysics, multiscale, and computational models for simulating the cardiac function

[03710] Virtual Populations of Heart Chimaeras: Generative Compositional Learning from Datasets of Datasets

[03238] The role of the Eikonal model in personalized cardiac modeling from parameter acquisition to arrhythmia simulations

[03521] An anisotropic eikonal model for cardiac repolarization and arrhythmias

[05281] Computational Models of Cardiac Electro-mechanical Function – Closing the Gaps between Virtual and Physical Reality

[04706] Scaling cardiac digital twins for population-based studies

[04251] A Local Space-Time Adaptive Scheme to Simulate Cardiac Electrophysiology

[03847] Parallel Performance of Robust and Scalable Multilevel Preconditioners in Cardiac Electrophysiology

[04140] Cardiac hemodynamics simulations with fluid-structure interaction and reduced valve modeling

[03773] Parametric Fluid-structure interaction solvers for haemodynamics

[04521] Towards developing high-speed cardiac mechanics simulations using a neural network finite element approach

[05099] Modeling Cardiac Fluid-Structure Interaction in the Human Heart

#### **[00710] Gender Equality in Mathematics: A Global Perspective**

[01733] Lessons on the global mathematical community from the 'Gender Gap in Science' global survey.

[02137] The African perspective about the Gender Gap in Science

[02048] gender diversity in Japanese concept

[02437] What we can do with Asian-Oceanian Women in Mathematics

[02658] Women in mathematics: an experience report and some facts about the European situation

[03111] Challenges for US Women in Math and the Activities of the AWM

[01795] The Standing Committee for Gender Equality in Science

[02912] Panel Discussion on Gender Equality

#### **[00711] Recent Advances in Optimal control and optimization**

[02838] PDE Constrained Optimization with Non-smooth Learning Informed Structures

[03725] Some optimal control problems in metric spaces

[03787] Exact controllability for systems describing plate vibrations. A perturbation approach.

[03789] A Perturbation Framework for Convex Minimization with Nonlinear Compositions

[03864] Analysis and Control in Poroelastic Systems

#### **[00715] Recent Trends in Market Design**

[01261] Fair division algorithms for house chores

[01327] Mechanism Design with Uncertainty

[01399] Best of Both Worlds in Fair Division

[01408] Strong Revenue (Non-)Monotonicity of Single-parameter Auctions

[01426] Tract housing, the core, and pendulum auctions

[01516] Are Simple Mechanisms Optimal when Agents are Unsophisticated?

[01530] Representation Theorems for Path-Independent Choice Rules

[01616] Optimal Dynamic Matching

[01620] Multi-Unit Bilateral Trade

[01693] Mechanism Design Powered by Social Interactions

[01738] Optimal allocation with costly verification and distributional constraint

[05446] Strategyproof Mechanisms for Group-Fair Facility Location Problems

#### **[00718] Data-driven and physics-informed techniques in Data Assimilation**

[02864] Consistency Results for some Bayesian PDE inverse problems

[05063] Data-driven and model-driven techniques in DA: applications, numerics, rigorous results

[02753] Nonparametric Bayesian inference of discretely observed diffusions

[02850] A general involution framework for Metropolis-Hastings algorithms and applications to Bayesian inverse problems

[02843] Insights from Nonlinear Continuous Data Assimilation for Turbulent Flows

[02852] Linear response for nonlinear dissipative SPDEs

[05078] Data assimilation of the 2D rotating NSE

[02847] Using machine learning in geophysical data assimilation (some of the issues and some ideas)

[02853] Almost Sure Error Bounds for Data Assimilation in Dissipative Systems with Unbounded Observation Noise

[04934] Challenges in high dimensional nonlinear filtering

[02745] Particle Filters for Data Assimilation

[04884] A novel regularity criterion for the 3D Navier-Stokes equations based on finitely many observations.

#### **[00719] Recent Advances in Numerical PDE and Scientific Machine Learning**

[04237] Level set learning for nonlinear dimensionality reduction in function approximation

[03271] Semi-analytic PINN methods for boundary layer problems on rectangular domains

[04847] Solving Wave Equations with Fourier Neural Operator

[04931] Physics-informed variational inference for stochastic differential equations

- [03076] Deep neural operator for learning transient response of composites subject to dynamic loading
- [05598] Analysis of the derivative-free method for solving PDEs using neural networks
- [03762] Convergence analysis of unsupervised Legendre-Galerkin neural networks for linear second-order elliptic PDEs
- [04540] Bi-orthogonal fPINN: A physics-informed neural network method for solving time-dependent stochastic fractional PDEs

**[00721] Data-driven and Model Reduction methods for Subsurface Applications**

- [04298] Deep Learning Methods for PDEs and Reduced Order Models
- [03429] Nonlocal multicontinua with representative volume elements
- [05249] Physics-informed neural networks for learning the homogenized coefficients of multiscale elliptic equations
- [02709] Optimality of statistical criterion in hyper-reduction
- [04174] Least-squares Method for Recovering Multiple Medium Parameters
- [03801] Adaptive partially explicit splitting scheme for multiscale flow problems

**[00727] Recent Advances in Fast Iterative Methods for PDE Problems**

- [02883] Multigrid Methods for Saddle-Point Matrices with Structured Blocks
- [05299] New Linear Solvers Features and Improvements in Trilinos
- [04769] A rational preconditioner for multi-dimensional Riesz fractional diffusion equations
- [02906] Some step-size independent theoretical bounds for preconditioning techniques of discrete PDEs
- [04605] A single-sided all-at-once preconditioning for linear system from a non-local evolutionary equation with weakly singular kernels
- [04933] Fast algorithms for space fractional Cahn-Hilliard equations
- [05262] A parallel preconditioner for the all-at-once linear system from evolutionary PDEs with Crank-Nicolson discretization in time
- [05468] A preconditioned MINRES method for optimal control of wave equations
- [03484] A block  $\alpha$ -circulant based preconditioned MINRES method for evolutionary PDEs

**[00731] Optimal control: methods and applications**

- [04845] A variational approach for modelling and optimal control of electrodynamic tether motion
- [04761] The Role of Stable Manifolds in Optimal Control under Stochastic Noise
- [04228] Second-order averaging of time-optimal low-thrust orbital transfers
- [03208] Optimization on manifolds by Riemannian gradient methods
- [04787] Curvature related properties of Finsler manifolds and applications
- [03504] Optimal microswimmer control and a microfluidic control example
- [04894] Control Problems inspired by Biological Phenomena
- [04045] Control in biology: topics in bacterial growth

**[00733] Compressible fluid dynamics and related PDE topics**

- [01289] Time-asymptotic stability of Riemann solutions to the compressible Navier-Stokes equations
- [01339] Stability analysis of Prandtl expansions for two dimensional MHD equations in Sobolev spaces
- [01378] Global Strong and Weak Solutions to Compressible MHD System
- [01436] Inviscid Limit Problem of radially symmetric stationary solutions for compressible Navier-Stokes equation
- [01614] Convergence Rate Estimates for the Low Mach and Alfvén Number Three-Scale Singular Limit of Compressible Ideal Magnetohydrodynamics
- [01617] Nonlinear asymptotic stability of vortex sheets with viscosity effects
- [01660] Time-asymptotic expansion with pointwise remainder estimates for 1D viscous compressible flow
- [01694] Asymptotic stability for the two-phase Navier-Stokes equations with surface tension and gravity
- [01716] Global solutions on compressible Euler and Euler-Poisson equations
- [01715] Global solutions on compressible Euler and Euler-Poisson equations
- [01776] Some recent results on compressible Navier-Stokes equations
- [03229] Hidden structures behinds the compressible Navier-Stokes equations and its applications to the corresponding models

**[00736] Modeling and Computation for Interface Dynamics in Fluids and Solids**

- [02231] Competition between viscous flow and diffusion in pinch-off dynamics
- [02273] A phase field model of vesicle growth or shrinkage
- [03394] A symmetrized parametric finite element method for anisotropic surface diffusion
- [02478] On a diffuse interface model for incompressible viscoelastic two-phase flows
- [03198] Simulating solid-state dewetting of thin films: a phase-field approach
- [03625] Modeling and simulation for solid-state dewetting problems
- [02975] Modeling and Energy Stable Numerical Schemes of Network Development in Biology Gels
- [03582] The mixed finite element method applied to cavitation in incompressible nonlinear elasticity

**[00737] Numerical methods for semiconductor devices simulation and the computational lithography**

- [01756] Arbitrarily high order finite element methods for arbitrarily shaped domains with automatic mesh generation
- [01921] An iterative method for inverse lithography problem with TV regularization
- [03833] A SOURCE TRANSFER DOMAIN DECOMPOSITION METHOD FOR MAXWELL'S EQUATIONS
- [01824] Numerical simulation for quantum transports in nano-semiconductor device
- [01985] An efficient iterative scheme for the coupled Schrödinger-Poisson equations
- [01922] Dispersion Analysis of CIP-FEM for Helmholtz Equation
- [01779] Efficient Simulation Algorithm for FinFET and Gate-All-Around FET
- [01757] A finite element method for the Schrödinger-Poisson model

**[00739] Inequalities and entropy with applications**

- [02362] Refined Hermite-Hadamard inequalities and their applications to some n variable means
- [02747] Generalization of Hermite-Hadamard Mercer Inequalities for Certain Interval Valued Functions
- [01760] Generalized spectral radius of operators and related inequalities
- [03970]  $q$ -deformation of Böttcher-Wenzel inequality
- [01998] The reduced quantum relative entropy
- [02970] On the quantum Tsallis relative entropy of real order
- [02482] On log-sum inequalities
- [02313] On certain properties of Shannon's Entropy
- [02721] The permutation entropy and its applications on full-scale compartment fire data
- [02772] A Spectral Analysis of The Correlated Random Walk
- [05367] On a class of k-entanglement witnesses
- [03537] Violation of Bell's Inequality by Classical Correlation via Adaptive Dynamics

**[00746] Variational methods for singularities and concentration on low dimensional sets**

- [04293] Ginzburg-Landau with Oblique Anchoring and Boojums
- [04158] Dipole removal for discrete energy minimizers
- [03999] From Volterra's dislocations to strain-gradient plasticity
- [01900] Harmonic dipoles in elasticity
- [03156] effective geometric motions of Ginzburg--Landau equations with potentials of high-dimensional wells
- [02113] Quasistatic evolution problems for models of geomaterials coupling plasticity and damage
- [04281] Liquid crystal colloids: from the electrostatic analogy to interaction energies
- [03855] Evolution of vector fields on flexible curves and surfaces

**[00747] Analysis and Numerics on Deep Learning Based Methods for Solving PDEs**

- [02903] Deep adaptive sampling for numerical PDEs
- [03007] Deep Learning for PDEs: Domain Decomposition and Adaptivity
- [03091] Bridging Traditional and Machine Learning-based Algorithms for Solving PDEs: The Random Feature Method
- [03011] On deep learning techniques for solving convection-dominated convection-diffusion equations
- [04381] Learning Functional Priors and Posteriors from Data and Physics
- [03134] AI for Combustion
- [03476] DOSnet as a Non-Black-Box PDE Solver: When Deep Learning Meets Operator Splitting
- [04359] Residual Minimization for PDEs: Failure of PINN and Implicit Bias
- [03475] Feature Flow Regularization: Improving Structured Sparsity in Deep Neural Networks
- [04428] Asymptotic-Preserving Neural Networks for Multiscale Time-Dependent Linear Transport Equations

**[00749] Recent Advances on Preconditioners and Fast Solvers for Nonlinear PDEs**

- [04011] Nonlinear FETI-DP domain decomposition methods combined with deep learning
- [03539] A quasi-Newton method with a secant-like diagonal approximation of Jacobian for symmetric sparse nonlinear equations
- [02038] Robustness and Adaptivity of Iterative Solvers
- [01782] Generalized multiscale finite element method for highly heterogeneous compressible flow
- [03859] Efficient Schwarz Preconditioning Techniques for Nonlinear Problems Using FROSCh
- [01916] BDDC Algorithms for Oseen problems with HDG Discretizations
- [02272] Fully implicit multi-physics solver for advanced fission nuclear power plant
- [01417] Recent advances on high-performance computing algorithms for patient-specific blood flow simulations
- [01407] Nonlinear Preconditioning Strategies Based on Residual Learning for PDEs
- [02019] ENO schemes with adaptive order for solving hyperbolic conservation laws
- [03281] Energy stable schemes for gradient flows based on the DVD method
- [01460] Scalable multilevel preconditioners for hybrid-DG discretizations of nonlinear cell-by-cell cardiac models

## [00023] Recent advances on application driven nonlinear optimization

**Session Time & Room :**

00023 (1/2) : 5B (Aug.25, 10:40-12:20) @F402

00023 (2/2) : 5C (Aug.25, 13:20-15:00) @F402

**Type :** Proposal of Minisymposium

**Abstract :** This minisymposium focuses on the new optimization techniques for application problems. Different application scenarios like machine learning and signal processing will be referred.

**Organizer(s) :** Cong Sun

**Classification :** 49M37, 65K05**Minisymposium Program :**

00023 (1/2) : 5B @F402

## [01318] A Unified Single-loop Alternating Gradient Projection Algorithm for Nonconvex-Concave and Convex-Nonconcave Minimax Problems

**Format :** Talk at Waseda University**Author(s) :** Zi Xu (Shanghai University)Huiling Zhang (Shanghai University)Guanghui Lan (Georgia Institute of Technology)

**Abstract :** Much recent research effort has been directed to the development of efficient algorithms for solving minimax problems with theoretical convergence guarantees due to the relevance of these problems to a few emergent applications. In this paper, we propose a unified single-loop alternating gradient projection (AGP) algorithm for solving smooth nonconvex-(strongly) concave and (strongly) convex-nonconcave minimax problems. AGP employs simple gradient projection steps for updating the primal and dual variables alternatively at each iteration. We show that it can find an  $\varepsilon$ -stationary point of the objective function in  $O(\varepsilon^{-2})$  (resp.  $O(\varepsilon^{-4})$ ) iterations under nonconvex-strongly concave (resp. nonconvex-concave) setting. Moreover, its gradient complexity to obtain an  $\varepsilon$ -stationary point of the objective function is bounded by  $O(\varepsilon^{-2})$  (resp.,  $O(\varepsilon^{-4})$ ) under the strongly convex-nonconcave (resp., convex-nonconcave) setting. To the best of our knowledge, this is the first time that a simple and unified single-loop algorithm is developed for solving both nonconvex-(strongly) concave and (strongly) convex-nonconcave minimax problems. Moreover, the complexity results for solving the latter (strongly) convex-nonconcave minimax problems have never been obtained before in the literature. Numerical results show the efficiency of the proposed AGP algorithm.

Furthermore, we extend the AGP algorithm by presenting a block alternating proximal gradient (BAPG) algorithm for solving more general multi-block nonsmooth nonconvex-(strongly) concave and (strongly) convex-nonconcave minimax problems. We can similarly establish the gradient complexity of the proposed algorithm under these four different settings.

## [01287] Accelerated ADMM-type Methods for Convex and Nonconvex Optimization Problems

**Format :** Talk at Waseda University**Author(s) :** Jianchao Bai (Northwestern Polytechnical University)

**Abstract :** In this talk, several accelerated stochastic and deterministic Alternating Direction Method of Multipliers, abbreviated as ADMM, are presented for solving separable convex optimization problems whose objective function is the sum of a possibly nonsmooth convex function and a smooth function which is an average of many component convex functions. We also show an advanced inexact accelerated ADMM for solving separable nonsmooth and nonconvex optimization problem. The convergence and complexity of these algorithms are discussed briefly, and a number of large-scale examples have verified the effectiveness of our algorithms compared with state-of-the-art first-order methods.

## [01284] On a special discrete phase constrained complex-field optimization problem

**Format :** Talk at Waseda University**Author(s) :** Cong Sun (Beijing University of Posts and Telecommunications)

**Abstract :** Reconfigurable intelligent surface (RIS) with discrete phase shifts aided wireless communication network is considered. The resource allocation problem of sum rate maximization with power constraints and discrete phase shifts is solved. The complicated objective function is approximated by its upper bound. The difficult orthogonal constraint is penalized to the objective function through Courant penalty function technique. Two algorithms are proposed for the approximated problem based on alternating direction of multipliers method and proximal gradient method, respectively. Simulations show that the two proposed algorithms achieve higher sum rate with significantly lower computational cost than the state of the art.

## [01368] Stochastic regularized Newton methods for nonlinear equations

**Format :** Talk at Waseda University**Author(s) :** Jiani Wang (Chinese Academy of Sciences)Xiao Wang (Peng Cheng Laboratory)Liwei Zhang (Dalian University of Technology)

**Abstract :** In this talk, we study finding zeros of nonlinear equations, whose exact function information is normally expensive to calculate but approximations can be easily accessed via calls to stochastic oracles. Based on inexact line search we propose a stochastic regularised Newton method and investigate its global convergence and local convergence rate. We also propose a variant of algorithm incorporating variance reduction scheme and we establish its sample complexity. We also report some numerical results.

00023 (2/2) : 5C @F402

## [01475] An Efficient Quadratic-Programming Relaxation Based Algorithm for Large-Scale MIMO Detection

**Format :** Talk at Waseda University

**Author(s) :** Ping-Fan ZHAO (Beijing Institute of Technology)Qing-Na LI (Beijing Institute of Technology)Wei-Kun CHEN (Beijing Institute of Technology)Ya-Feng LIU (Academy of Mathematics and Systems Science, Chinese Academy of Sciences)

**Abstract :** Massive MIMO has been recognized as a key technology in 5G and beyond communication networks, which can significantly improve the communication performance, but also poses new challenges of solving the corresponding optimization problems due to the large problem size. In this talk, we propose an efficient sparse QP relaxation based algorithm for solving the large-scale MIMO detection problem. With exact recovery guaranteed, the algorithm achieves better detection performance compared with the state-of-art algorithms.

## [01487] Uniform Framework of Convergence Analysis for Nesterov's Accelerated Gradient Method

**Format :** Talk at Waseda University

**Author(s) :** Shuo Chen (Academy of Mathematics and Systems Science, Chinese Academy of Sciences)

**Abstract :** Nesterov's accelerated gradient method (**NAG**) is one of the most influenced methods used in machine learning and other fields. In this talk, we give a new framework to analyze convergence property of **NAG** based on the high-resolution differential equation, phase-space representation and Lyapunov functions. New convergence rate for gradient norm is revealed in convex case, while the requirement for stepsize is loosed and the convergence rate is improved for strongly convex objective.

## [01285] Exact continuous relaxations and algorithms for regularized optimization problems

**Author(s) :** Wei Bian (Harbin Institute of Technology)

**Abstract :** In this talk, we consider two classes of regularized optimization problems, in which the group sparsity is considered. Firstly, we give the continuous relaxation models of the considered problem and establish the equivalence of these two problems in the sense of global minimizers. Then, we define a class of stationary points of the relaxation problem, and prove that any defined stationary point is a local minimizer of the considered regularized problem and satisfies a desirable property of its global minimizers. Further, based on the difference-of-convex (DC) structure of the relaxation problem, we design some corresponding algorithms and prove their convergence properties.

# [00024] Geometric methods in machine learning and data analysis

**Session Time & Room :**

00024 (1/3) : 1C (Aug.21, 13:20-15:00) @G709

00024 (2/3) : 1D (Aug.21, 15:30-17:10) @G709

00024 (3/3) : 1E (Aug.21, 17:40-19:20) @G709

**Type :** Proposal of Minisymposium

**Abstract :** Geometry plays a paramount role in many aspects of data analysis and machine learning: Graphs on high-dimensional datasets encode interactions between geometry and data; Geometries on the space of probability measures give rise to new optimization and sampling algorithms; Geometric deep learning translates deep learning to new domains; Adversarial regularization of neural networks corresponds to geometric regularization. In this minisymposium we gather junior and senior researchers who have been driving the research in the field, using geometric methods for both analysis and algorithms. We aim at sparking new collaborations in this vibrant field and offering a platform for scientific exchange.

**Organizer(s) :** Leon Bungert, Jeff Calder

**Classification :** 35R02, 68T05, 49Q22

**Minisymposium Program :**

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00024 (1/3) : 1C @G709 [Chair: Leon Bungert]

## [03148] Geometric Data Analysis via Discrete Curvature

**Format :** Talk at Waseda University

**Author(s) :** Melanie Weber (Harvard University)

**Abstract :** The problem of identifying geometric structure in heterogeneous, high-dimensional data is a cornerstone of Machine Learning. In this talk, we approach this problem from the perspective of Discrete Geometry. We begin by reviewing discrete notions of curvature, where we focus especially on discrete Ricci curvature. Then we consider a setting, where a given point cloud was sampled from an (unknown) manifold. We give pointwise consistency results for the discrete curvature of a geometric graph build from the point cloud and the curvature of the manifold. We further show that if the manifold has curvature bounded from below by a positive constant, the geometric graph will inherit this global structural property with high probability. Finally, we discuss applications of discrete curvature and our consistency results in Geometric Data Analysis, including graph-based clustering and regression. The talk is based on joint work with Nicolas Garcia Trillos, Zachary Lubberts and Yu Tian.

## [02978] Large data limit of the MBO scheme for data clustering

**Format :** Online Talk on Zoom

**Author(s) :** Jona Lelmi (University of Bonn)Tim Laux (University of Bonn)

**Abstract :** The MBO scheme is a highly performant scheme used for data clustering. Given some data, one constructs the similarity graph associated with the data points. The goal is to split the data into meaningful clusters. The algorithm produces the clusters by alternating between diffusion on the graph and pointwise thresholding. In this talk, I will present the first theoretical studies of the scheme in the large data limit. We will see how the final state of the algorithm is asymptotically related to minimal surfaces in the data manifold and how the dynamic of the scheme is asymptotically related to the trajectory of steepest descent for surfaces, which is mean curvature flow. The tools employed are variational methods and viscosity solutions techniques. Based on joint work with Tim Laux (U Bonn).

## [03210] Topologies of convergences for discrete-to-continuum limit on Poission point clouds

**Format :** Talk at Waseda University

**Author(s) :** Marco Caroccia (Politecnico di Milano)

**Abstract :** Energies on point clouds have attracted increasing attention in the last decades, especially due to their application to machine learning and data analysis. What seems to arise from the collection of the results at several scales is that a change in the topology of Gamma-convergence occur when the point clouds is connected at a very short-range interaction scale. Typically, in literature, the interaction range considered is big enough to neglect the defects arising from the stochastic geometry of the point clouds. In the small range interaction regime instead the geometry of the point clouds

cannot be neglected in the analysis of the discrete-to-continuum limit. We will present the various topologies of convergence and the different techniques that are required to obtain the discrete-to-continuum limit at different scales.

## [03219] Spectral Methods for Data Sets of Mixed Dimensions

**Format :** Talk at Waseda University

**Author(s) :** Leon Bungert (Technical University of Berlin)Dejan Slepcev (Carnegie Mellon University)

**Abstract :** High dimensional data often consist of parts with different intrinsic dimension. We study how spectral methods on graphs adapt to data containing intersecting pieces of different dimensions. We show that unnormalized Laplacian strongly prefer the highest dimension, while appropriately normalized Laplacian converges to Laplace-Beltrami operator in all dimensions simultaneously. For intersecting manifolds we identify when and how is the information transferred between manifolds.

00024 (2/3) : 1D @G709 [Chair: Jeff Calder]

## [03228] An information geometric and optimal transport framework for Gaussian processes

**Format :** Talk at Waseda University

**Author(s) :** Minh Ha Quang (RIKEN Center for Advanced Intelligence Project)

**Abstract :** Information geometry (IG) and Optimal transport (OT) have been attracting much research attention in various fields, in particular machine learning and statistics. In this talk, we present results on the generalization of IG and OT distances for finite-dimensional Gaussian measures to the setting of infinite-dimensional Gaussian measures and Gaussian processes. Our focus is on the Entropic Regularization of the 2-Wasserstein distance and the generalization of the Fisher-Rao distance and related quantities. In both settings, regularization leads to many desirable theoretical properties, including in particular dimension-independent convergence and sample complexity. The mathematical formulation involves the interplay of IG and OT with Gaussian processes and the methodology of reproducing kernel

part\_1

Hilbert spaces (RKHS). All of the presented formulations admit closed form expressions that can be efficiently computed and applied practically. The theoretical formulations will be illustrated with numerical experiments on Gaussian processes.

## [03101] Data analysis and optimal transport: some statistical tools

**Format :** Talk at Waseda University

**Author(s) :** Elsa Cazelles (CNRS, Université de Toulouse)

**Abstract :** We focus on the analysis of data that can be described by probability measures supported on a Euclidean space, through optimal transport. Our main objective is to present first and second order statistical analyses in the space of distributions, as a first approach to understand the general modes of variation of a set of observations. These studies correspond to the barycenter and the decomposition into geodesic principal components in the Wasserstein space.

## [02871] Multispecies Optimal Transport and its Linearization

**Format :** Talk at Waseda University

**Author(s) :** Katy Craig (Department of Mathematics at the University of California Santa Barbara)Nicolás García Trillo (Department of Statistics at the University of Wisconsin Madison)Dorde Nikolic (Department of Mathematics at the University of California Santa Barbara)

**Abstract :** The discovery of linear optimal transport by Wang et al. in 2013 improved the computational efficiency of optimal transport algorithms for grayscale image classification. Our main goal is to classify multicolor images arising in collider events. We will introduce the basics of linear optimal transport theory, and the multispecies distance. I will discuss similarities of the multispecies case with the Hellinger-Kantorovich distance, which was linearized in 2021 by Cai et al., via its Riemannian structure.

## [03196] Semi-supervised learning with the p-Laplacian

**Format :** Talk at Waseda University

**Author(s) :** Nadejda Drenska (Louisiana State University)Jeff Calder (University of Minnesota, Twin Cities)

**Abstract :** Semi-supervised learning involves learning from both labeled and unlabeled data. In this talk we apply p-Laplacian regularization to cases of very low labeling rate; in such applications this approach classifies properly when the standard Laplacian regularization does not. Using the two-player stochastic game interpretation of the p-Laplacian, we prove asymptotic consistency of p-Laplacian regularized semi-supervised learning, thus justifying the utility of the p-Laplacian.

This is joint work with Jeff Calder.

00024 (3/3) : 1E @G709 [Chair: Leon Bungert]

## [03217] The passive symmetries of machine learning

**Format :** Talk at Waseda University

**Author(s) :** Soledad Villar (Johns Hopkins University)

**Abstract :** Any representation of data involves arbitrary investigator choices. Because those choices are external to the data-generating process, each choice leads to an exact symmetry, corresponding to the group of transformations that takes one possible representation to another. These are the passive symmetries; they include coordinate freedom, gauge symmetry and units covariance, all of which have led to important results in physics. Our goal is to understand the implications of passive symmetries for machine learning: Which passive symmetries play a role (e.g., permutation symmetry in graph neural networks)? What are dos and don'ts in machine learning practice? We assay conditions under which passive symmetries can be implemented as group equivariances. We also discuss links to causal modeling, and argue that the implementation of passive symmetries is particularly valuable when the goal of the learning problem is to generalize out of sample.

## [03186] Graphons in Machine Learning

**Format :** Talk at Waseda University

**Author(s) :** Luana Ruiz (Johns Hopkins University)

**Abstract :** Graph neural networks are successful at learning representations from graph data but suffer from limitations in large graphs. Yet, large graphs can be identified as being similar to each other in the sense that they share structural properties. Indeed, graphs can be grouped in families converging to a common graph limit--- the graphon. In this talk, I discuss how graphons can be used to lay the theoretical foundations for machine learning on large-scale graphs.

## [03178] Graphon Analysis of Graph Neural Networks

**Format :** Talk at Waseda University

**Author(s) :** Ron Levie (Technion - Israel Institute of Technology)

**Abstract :** In recent years, graph neural networks have led to ground-breaking achievements in the applied sciences and industry. These achievements pose exciting theoretical challenges: can the success of graph neural networks (GNNs) be grounded in solid mathematical frameworks?

In this talk, I will show how to define GNN input domains using graphon analysis, and how such domains lead to a universal analysis of GNNs, with generalization bounds and approximation theorems.

## [03202] Graph Neural Networks on Large Random Graphs: Convergence, Stability, Universality

**Format :** Talk at Waseda University

**Author(s) :** Nicolas Keriven (CNRS, IRISA)

**Abstract :** In this talk, we will discuss some theoretical properties of GNNs on large graphs. We assume that the graphs are generated with classical models of random graphs. We characterize the convergence of GNNs as the number of nodes grows. We study their stability to small deformations of the underlying model, a crucial property in traditional CNNs. Finally, we study their approximation power, and show how some recent GNNs are more powerful than others.

# [00027] Recent trends on crowd management

**Session Time & Room :** 3E (Aug.23, 17:40-19:20) @A208

**Type :** Proposal of Minisymposium

**Abstract :** Crowd management is an interdisciplinary field that has received much attention in recent year, and various scientific methods for reducing the risk of crowd avalanches and infections are being studied. In addition, encouraging decentralized behavior not only enhances safety, but also improves services from marketing viewpoints. Latest research results on sensing, simulation and guidance of crowds, which are all very important in crowd management, will be discussed by applied mathematicians from different backgrounds.

**Organizer(s) :** Katsuhiro Nishinari, Claudio Feliciani, Kensuke Yasufuku ,Tetsuya Aiko

**Classification :** 91C05, 00A71, 62P25, 68U07, 62P15

**Minisymposium Program :**

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00027 (1/1) : 3E @A208 [Chair: Katsuhiro Nishinari]

## [05480] Crowd Management Platform as a Service

**Format :** Talk at Waseda University

**Author(s) :** Katsuhiro Nishinari (The University of Tokyo)

**Abstract :** Crowd management is important for safety and efficient movement of individuals. The process involves sensing crowd conditions in real time, predicting the near future from that data, and then guiding the crowd through a risk assessment to prevent accidents before they happen. The platform supporting this series of functions is named Crowd Management Platform as a Service (CMPaaS).In the presentation, actual case studies using CMPaaS will be presented.

## [05405] 3D Visualization of Crowd Motion

**Format :** Online Talk on Zoom

**Author(s) :** Kensuke Yasufuku (Osaka University)

**Abstract :** This presentation proposes methods for effective 3D visualization of crowd motion in large sites under both normal and emergency conditions. We utilize agent-based crowd simulations to model and predict behavioral patterns under various scenarios. These simulations serve as critical tools for predicting congestion within these sites and for evaluating and optimizing appropriate evacuation plans. Furthermore, we will discuss visualization techniques for sharing information among stakeholders.

## [05377] Numerical description of pedestrian crowds: are we really particles?

**Format :** Talk at Waseda University

**Author(s) :** Claudio Feliciani (The University of Tokyo)

**Abstract :** Quantification of properties related to pedestrian crowds is necessary for analyzing pedestrian flows and automating real-time control. Often, models inspired by physics and fluid dynamics are used to describe crowds by simplifying people as particles. While these models often yield good results, they are typically only valid for specific conditions. This highlights the need to better understand the cognitive and psychological aspects of human motion in crowds to improve the quantification of pedestrian collective dynamics.

## [05404] Crowd management and visitors' attitudes in natural recreational areas

**Format :** Talk at Waseda University

**Author(s) :** Tetsuya Aikoh (Hokkaido University) Hyerin Kim (Hokkaido University) Yasushi Shoji (Hokkaido University)

**Abstract :** While outdoor recreation areas are expected to attract visitors, there are concerns about overtourism. Outdoor spaces without obvious entrances and exits present many sensing challenges. In addition, controlling crowding in public recreation areas requires consensus with visitors and local stakeholders. We will report on recent research findings and their contribution to management in World Heritage areas and urban greening events.

# [00029] New Trends in Structural and Engineering Optimization

**Session Time & Room :**

00029 (1/2) : 4E (Aug.24, 17:40-19:20) @A508

00029 (2/2) : 5C (Aug.25, 13:20-15:00) @A508

**Type :** Proposal of Minisymposium

**Abstract :** Over a wide range of modern engineering design, numerical optimization plays crucial roles in diverse decision-making processes. This minisymposium aims to bring together recent advances in various aspects of structural and engineering optimization. The topics of interest include, but are not limited to

- new advances in structural optimization methods,
- surrogate modeling and digital twins for engineering optimization,
- multi-scale and microstructural topology optimization,
- machine learning and data-driven approaches to optimization.

**Organizer(s) :** Yoshihiro Kanno, Satoshi Kitayama, Akihiro Takezawa

**Classification :** 90C90, 65K10, 49M37, 74P05, 74P10

**Minisymposium Program :**

00029 (1/2) : 4E @A508 [Chair: Satoshi Kitayama]

## [04641] Topology optimization reducing the dynamic instability of squeal noise

**Format :** Talk at Waseda University

**Author(s) :** SolJi Han (Hanyang University) GilHo Yoon (hanyang university)

**Abstract :** This study focuses on topology optimization considering the dynamic instability of squeal noise. In this study, the instability value caused by the frictional force is analysed through the eigenvalue analysis, and the sensitivity is calculated by left and right eigenvectors. With the present development, it is possible to optimize a structure that effectively reduces the instability value. To verify this study, several optimization examples are considered.

## [03974] Structural simulation and optimization to improve the quality of metal additive manufacturing

**Format :** Talk at Waseda University

**Author(s) :** Akihiro Takezawa (Waseda University)

**Abstract :** Reduction of the residual warpage generated through fabrication is an emerging issue in metal laser powder bed fusion additive manufacturing (AM). Regarding the minimization of the residual warpage of the lattice infill structures, simultaneous optimization of the laser hatching orientation and lattice density distribution is conducted in this study to confirm their synergetic effect.

## [03594] Machine-learning assisted topology optimization with structural gene inheritance

**Format :** Talk at Waseda University

**Author(s) :** Weisheng Zhang (Dalian University of Technology) Sung-Kie Youn (KAIST) Xu Guo (Dalian University of Technology)

**Abstract :** A machine-learning assisted topology optimization approach is proposed for structural design with structural gene inheritance. This work establishes a novel framework to systematically integrate structural topology optimization with subjective human design preferences. To embed the structural gene into the design, neural style transfer technique is adopted to measure and generate the prior knowledge from a reference image with the concerned structural gene (such as biological characteristic, artistic flavor and manufacturing requirement, etc.). By using different convolutional layers in the VGG-19 model-based CNN, both the style and content of the structural gene can be constructed from low to high levels of abstraction. The measured knowledge can then be integrated into pixel-based topology optimization as a formal similarity constraint. Both 2D and 3D problems are solved to illustrate the effectiveness of the proposed approach where the inheritance of the structural gene can be achieved in a systematic manner.

00029 (2/2) : 5C @A508 [Chair: Akihiro Takezawa]

## [03346] Numerical and experimental investigation on process parameters optimization in rapid heat cycle molding

**Format :** Talk at Waseda University

**Author(s) :** Satoshi Kitayama (Kanazawa University) Yusuke Yamazaki (Sodick Co. Ltd.) Yoshikazu Kubo (Sodick Co. Ltd.) Shuji Aiba (Sodick Co. Ltd.)

**Abstract :** Weldline that forms when two or more melt fronts meet is one of the major defects in plastic injection molding (PIM), and it is important to reduce the weldline as much as possible. Rapid heat cycle molding (RHCM) is one of the effective PIMs for weldline reduction, but the process parameters are determined by the trial and error method. This paper optimizes the process parameters in RHCM by CAE and design optimization technique. The experiment is also conducted to examine the validity of the proposed approach.

## [01219] Acoustic metamaterials design with non-gradient material-field series-expansion topology optimization

**Format :** Talk at Waseda University

**Author(s) :** Xiaopeng Zhang (Dalian University of Technology) University of Technology

**Abstract :** Designing bandgap acoustic metamaterial has important application potential but is also challenging. This study proposes a systematic topology optimization method of acoustic metamaterial to open single and multiple low-frequency bandgaps. To describe the complicated topologies of the multi-material acoustic metamaterial with a lower number of design variables, the material-field series expansion (MFSE) technique is adopted. With the interpolated scheme and the multi-material field description model, a clear three-material topology can be determined by two independent material-field functions with only 100 independent design variables. This greatly reduces the design variables for the topological description of the microstructure, enabling the problem to be solved using non-gradient optimization algorithms. The self-adaptive strategy based sequential Kriging optimization algorithm is then introduced to solve the optimization problems. Numerical examples prove the proposed topology optimization method can effectively provide the acoustic metamaterial designs with ultra-wide low-frequency bandgaps.

## [04675] Multiscale topology optimization to maximize dissipated energy

**Format :** Talk at Waseda University

**Author(s) :** Takashi Yamamoto (Kogakuin University)

**Abstract :** In this study, a multiscale topology optimization method for micro structure is proposed utilizing the homogenization method based on the asymptotic expansion. Energy dissipated in macroscopic component is maximized at a prescribed frequency. Design sensitivities of the homogenized macroscopic properties are calculated by applying the

adjoint variable method in the frame work of the homogenization method. Adjoint variable method is hierarchically applied to obtain design sensitivities of the macroscopic dissipated energy.

## [03135] Multiscale topology optimization of fiber reinforced composite using homogenization design method.

**Format :** Talk at Waseda University

**Author(s) :** Jaewook Lee (Gwangju Institute of Science and Technology (GIST))

**Abstract :** This presentation shows topology optimization of fiber reinforced composite with spatially-varying fiber structure. The numerical homogenization of the microscale unit-cell is performed at various fiber sizes. Then, the effective elasticity tensor is represented as the function of fiber size and orientations, together with the density. Topology optimization is carried out at macroscale, and the microscale composite structure is restored using the de-homogenization method. Both 2D and 3D design examples will be provided.

## [00033] Recent Advances on Quantitative Finance

**Session Time & Room :**

00033 (1/3) : 5B (Aug.25, 10:40-12:20) @A510

00033 (2/3) : 5C (Aug.25, 13:20-15:00) @A510

00033 (3/3) : 5D (Aug.25, 15:30-17:10) @A510

**Type :** Proposal of Minisymposium

**Abstract :** The mini-symposium we propose aims to feature the latest developments and promote research in the field of quantitative finance. The mini-symposium will enhance interaction and cooperation among researchers worldwide working on some specific topics in the field. In particular, we will focus on, but are not limited to, the following three topics:

- stochastic control in quantitative finance,
- dynamic game and mean-field game in quantitative finance, and
- machine learning and reinforcement learning in quantitative finance.

Consequently, we plan to have three sessions on the above three topics, respectively

**Organizer(s) :** Min Dai, Zuoquan Xu, Chao Zhou  
**Sponsor :** This session is sponsored by the SIAM Activity Group on Financial Mathematics and Engineering.

**Classification :** 91G10, 93E20, 35Q91, 49N90

**Minisymposium Program :**

00033 (1/3) : 5B @A510 [Chair: Min Dai]

## [04926] Neural Stopping Boundaries

**Format :** Talk at Waseda University

**Author(s) :** Halil Mete Soner (Princeton University)Anders Max Reppen (Boston University Questrom School of Business)Valentin Tissot-Daguette (Princeton University)

**Abstract :** A method based on deep artificial neural networks and empirical risk minimization is developed to calculate the boundary separating the stopping and continuation regions in optimal stopping. The algorithm parameterizes the stopping boundary as the graph of a function and introduces relaxed stopping rules based on fuzzy boundaries to facilitate efficient optimization. Several examples related to financial instruments, some in high dimensions, are analyzed through this method, demonstrating its effectiveness. The existence of the stopping boundary is also proved under natural structural assumptions. We also briefly show how this method applies to the classical Stefan problem of solidification.

## [05322] Learning Equilibrium Mean-Variance Strategy

**Format :** Talk at Waseda University

**Author(s) :** Min Dai (The Hong Kong Polytechnic University)Yuchao Dong (Tongji University)Yanwei Jia (Columbia University)

**Abstract :** We study a dynamic mean-variance portfolio optimization problem under the reinforcement learning framework,

where an entropy regularizer is introduced to induce exploration. Due to the time-inconsistency involved in a mean-variance criterion, we aim to learn an equilibrium policy. Under an incomplete market setting, we obtain a semi-analytical, exploratory, equilibrium mean-variance policy that turns out to follow a Gaussian distribution. We then focus on a Gaussian mean return model and propose a reinforcement learning algorithm to find the equilibrium policy. Thanks to a thoroughly designed policy iteration procedure in our algorithm, we prove the convergence of our algorithm under mild conditions, despite that dynamic programming principle and the usual policy improvement theorem failing to hold for an equilibrium policy. Numerical experiments are given to demonstrate our algorithm. The design and implementation of our reinforcement learning algorithm apply to a general market setup.

## [05301] On Consistency of Selecting Signatures Using Lasso: A Tale of Ito and Stratonovich

**Format :** Talk at Waseda University

**Author(s) :** Xin Guo (UC Berkeley)Ruixun Zhang (Peking University)Chaoyi Zhao (Peking University)

**Abstract :** We investigate the statistical consistency of using Lasso to select signatures in machine learning predictions. Signatures are defined as iterated path integrals of stochastic processes, and their universal nonlinearity warrants Lasso as a common tool to select sparse linear approximations. We study the consistency of Lasso for selecting signatures for the Brownian motion, the Ornstein–Uhlenbeck process, and the fractional Brownian motion, both theoretically and numerically. Our findings show that, for signatures defined by Ito integrals, Lasso is more consistent for processes that are closer to Brownian motion and have weaker inter-dimensional correlations. For signatures defined by Stratonovich integrals, we observe better Lasso consistency for mean-reverting processes than for mean-averting processes. Our results emphasize the importance of choosing appropriate definitions of signatures in statistical inference and machine learning, particularly for non-Brownian processes.

## [02766] Portfolio choice with transaction costs and reinforcement learning

**Format :** Talk at Waseda University

**Author(s) :** Min Dai (Hong Kong Polytechnic University)

**Abstract :** We provide a reinforcement learning approach for portfolio choice with transaction costs. Numerical results are provided to demonstrate the efficiency of our approach.

00033 (2/3) : 5C @A510 [Chair: Zuoquan Xu]

## [05335] Dynamic programming for mean-variance portfolio selection

**Format :** Talk at Waseda University

**Author(s) :** Martin Schweizer (ETH Zurich)

**Abstract :** We present a dynamic programming approach to solving the mean-variance portfolio selection problem in finite discrete time. This bypasses issues of time-inconsistency and hence does not need the introduction of an equilibrium or game-theoretic approach. The talk is based on joint work with Zhouyi Tan.

## [05363] Non-Concave Utility Maximization with Transaction Costs

**Format :** Talk at Waseda University

**Author(s) :** shuaijie qian (Hong Kong University of Science and Technology)Chen Yang (The Chinese University of Hong Kong)

**Abstract :** We consider the non-concave utility maximization problem, which appears in plenty of areas in finance, with transaction costs. Technically, we propose a proper terminal condition and lay the corresponding theoretical foundation of viscosity solutions. This terminal condition implies that any transaction close to maturity provides a marginal contribution to the target. We find that the introduction of transaction costs into non-concave utility problems can prevent the portfolio from unbounded leverage and also result in richer action regions than classical transaction costs problems with concave utilities.

## [05320] Optimal stopping without time consistency

**Format :** Talk at Waseda University

**Author(s) :** Hanqing Jin (University of Oxford)Yanzhao Yang (University of Oxford)

**Abstract :** We study a continuous time dynamic optimal stopping problem with a flow of preferences, which can be in non-expectation form and can depend on both the current time and state of the system in general. We will define a solution to the problem by the rationality of the agent, and compare it with other solutions appeared in literature.

## [03404] Optimal dividend payout with non-decreasing constraint

**Format :** Talk at Waseda University

**Author(s) :** Zuo Quan Xu (The Hong Kong Polytechnic University)Chonghu Guan (Jiaying University)

**Abstract :** We study a dividend payout problem under the classical Cram'er-Lundberg model. The dividend payout must be non-decreasing over time and is subject to an upper bound constraint. Finding the optimal dividend payout strategy in this model is a long-standing open problem in risk theory. To overcome the difficulty, we first introduce a regime-switching problem --- a sequence of single-obstacle problems in ODE --- to approximate the original two-dimensional HJB equation and then take limit. We find a smooth switching boundary and the optimal strategy is given by the boundary.

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00033 (3/3) : 5D @A510 [Chair: Chao Zhou]

## [05500] Extended mean-field control problems with multi-dimensional singular controls

**Format :** Talk at Waseda University

**Author(s) :** Ulrich Horst (Humboldt University Berlin)Robert Denkert (Humboldt University Berlin)

**Abstract :** We consider extended mean-field control problems with multi-dimensional singular controls. A key challenge when analysing singular controls are jump costs. When controls are one-dimensional, jump costs are most naturally computed by linear interpolation. When the controls are multi-dimensional the situation is more complex, especially when the model parameters depend on an additional mean-field interaction term, in which case one needs to "jointly" and consistently" interpolate jumps both on a distributional and a pathwise level. This is achieved by introducing the novel concept of two-layer parametrisations of stochastic processes. Two-layer parametrisations allow us to equivalently rewrite rewards in terms of continuous functions of parametrisations of control process and to derive an explicit representation of rewards in terms of minimal jump costs. From this we derive a DPP for extended mean-field control problems with multi-dimensional singular controls. Under the additional assumption that the value function is continuous we characterise the value function as the minimal super-solution to a certain quasi-variational inequality in the Wasserstein space.

## [05172] Lightning Network Economics: Channels and Topology

**Format :** Talk at Waseda University

**Author(s) :** Paolo Guasoni (Dublin City University)Gur Huberman (Columbia Business School)Clara Shikhelman (Chaincode Labs)

**Abstract :** Designed to address Bitcoin's scalability challenge, the Lightning Network (LN) is a protocol allowing two parties to secure bitcoin payments and escrow holdings between them. In a lightning channel, each party commits collateral towards future payments to the counterparty and payments are cryptographically secured updates of collaterals. First, we identify conditions for two parties to optimally establish a channel, find explicit formulas for channel costs and optimal collaterals, and derive the implied reduction in congestion of the blockchain. Then we obtain necessary conditions for cost-minimizing topologies and bounds on the cost of the optimal topology, showing the unusual circumstances in which it is a hub that connects all other nodes.

## [05309] Non-monotone linear-quadratic mean field games with a major player

**Format :** Talk at Waseda University

**Author(s) :** Chenchen Mou (City University of Hong Kong)Min Li (Shandong University)Zhen Wu (Shandong University)Chao Zhou (National University of Singapore)

**Abstract :** In this talk, we consider a class of linear-quadratic mean field games with a major player. The game has the feature that the major player can have an impact on all the minor players while the minor players as a whole influence the major player. The value functions corresponding to the major and minor players satisfy the corresponding master equations, which generate the so-called master system. To the best of our knowledge, the global wellposedness of the master system remains open. The main focus of the paper is to tackle the open problem in the linear-quadratic setting without any monotonicity conditions. The key idea is to use the non-degeneracy of the common noise to show the global wellposedness of the Nash certainty equivalence system for the minor players. Meanwhile, we also study the corresponding  $N$ -minor player and a major player game. More precisely, we show the quantitative convergence from the  $N$ -minor player and a major player game to the mean field game and the propagation of chaos property for the related optimal trajectories for both the minor players and the major player. This is based on a joint work with M. Li, Z. Wu and C. Zhou.

## [05501] Large ranking games with diffusion control

**Format :** Talk at Waseda University

**Author(s) :** Stefan Ankirchner (University of Jena)Nabil Kazi-Tani (Université de Lorraine)Julian Wendt (University of Jena)Chao Zhou (National University of Singapore)

**Abstract :** We consider a symmetric stochastic differential game where each player can control the diffusion intensity of an individual dynamic state process, and the players whose states at a deterministic finite time horizon are among the best  $\alpha \in (0, 1)$  of all states receive a fixed prize. Within the mean field limit version of the game we compute an explicit equilibrium, a threshold strategy that consists in choosing the maximal fluctuation intensity when the state is below a given threshold, and the minimal intensity else. We show that for large  $n$  the symmetric  $n$ -tuple of the threshold strategy provides an approximate Nash equilibrium of the  $n$ -player game. We also derive the rate at which the approximate equilibrium reward and the best response reward converge to each other, as the number of players  $n$  tends to infinity. Finally, we compare the approximate equilibrium for large games with the equilibrium of the two player case.

## [00036] Different perspectives in non-linear and non-local PDEs

**Session Time & Room :**

00036 (1/3) : 1C (Aug.21, 13:20-15:00) @G602

00036 (2/3) : 1D (Aug.21, 15:30-17:10) @G602

00036 (3/3) : 1E (Aug.21, 17:40-19:20) @G602

**Type :** Proposal of Minisymposium

**Abstract :** The aim of this minisymposium is to gather researchers involved in the mathematical analysis of non-linear and non-local partial differential equations (PDEs), with emphasis on those modelling aggregation and/or diffusion phenomena. These PDEs are relevant in applications to physics, biology, population dynamics, data science, etc. The spectrum of possible mathematical approaches involves techniques from functional analysis, optimal transport theory, variational methods, etc. It is at the core of our minisymposium to touch upon recent advances in the study of aggregation-diffusion PDEs obtained, e.g., using generalised gradient flows, incompressible limits, particle approximations, numerical methods, symmetrisation and rearrangements, and Fourier analysis.

**Organizer(s) :** Antonio Esposito, David Gómez-Castro

**Classification :** 35K55, 35K65, 35B40, 35Q70, 35A15

**Minisymposium Program :**

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00036 (1/3) : 1C @G602 [Chair: Antonio Esposito]

## [04031] Quantified overdamped limit for Vlasov-Fokker-Planck equations with singular interaction forces

**Format :** Talk at Waseda University

**Author(s) :** Young-Pil Choi (Yonsei University)

**Abstract :** In this talk, I will discuss a quantified overdamped limit for kinetic Vlasov-Fokker-Planck equations with nonlocal interaction forces. We provide explicit bounds on the error between solutions of that kinetic equation and the limiting equation, which is known under the names of aggregation-diffusion equation or McKean-Vlasov equation. Our strategy only requires weak

integrability of the interaction potentials, thus in particular it includes the quantified overdamped limit of the kinetic Vlasov-Poisson-Fokker-Planck system to the aggregation-diffusion equation with either repulsive electrostatic or attractive gravitational interactions.

## [04055] A Degenerate Cross-Diffusion System as the Inviscid Limit of a Nonlocal Tissue Growth Model

**Format :** Talk at Waseda University

**Author(s) :** Noemi David (University of Lyon)Tomasz Dębiec (University of Warsaw)Mainak Mandal (Technische Universität Dresden)Markus Schmidtchen (Technische Universität Dresden)

**Abstract :** In recent years, there has been a spike in interest in multi-phase tissue growth models. Depending on the type of tissue, the velocity is linked to the pressure through Stoke's law, Brinkman's law or Darcy's law. While each of these velocity-pressure relations has been studied in the literature, little emphasis has been placed on the fine relationship

between them. In this paper, we want to address this dearth in the literature, providing a rigorous argument that bridges the gap between a viscoelastic tumour model (of Brinkman type) and an inviscid tumour model (of Darcy type).

## [03802] Nonlocal particle approximations of the porous medium equation

**Format :** Online Talk on Zoom

**Author(s) :** Katy Craig (University of California, Santa Barbara)Olga Turanova (Michigan State University)Karthik Elamvazhuthi (University of California, Riverside)Matt Haberland (Cal Poly, San Luis Obispo)

**Abstract :** Given a desired target distribution and an initial guess of its samples, what is the best way to evolve the locations of the samples so that they accurately represent the desired distribution? A classical solution to this problem is to evolve the samples according to Langevin dynamics, a stochastic particle method for the Fokker-Planck equation. In today's talk, I will contrast this with a nonlocal, deterministic particle method inspired by the porous medium equation. Using the Wasserstein gradient flow structure of the equations and Serfaty's scheme of Gamma-convergence of gradient flows, I will show that, as the number of samples increases and the interaction scale goes to zero, the interacting particle system indeed converges to a solution of the porous medium equation. I will close by discussing practical implications of this result to both sampling and the training dynamics two-layer neural networks. This is based on joint work with Karthik Elamvazhuthi, Matt Haberland, and Olga Turanova.

## [05056] A convergent discretization of the porous medium equation with fractional pressure

**Format :** Talk at Waseda University

**Author(s) :** Félix del Teso (Universidad Autónoma de MadridU)

**Abstract :** We carefully construct and prove convergence of what is to our knowledge the first numerical discretization of the porous medium equation with fractional pressure,

$$\begin{aligned} \begin{array}{l} \text{\begin{equation}\text{\tag{FPE}}\end{equation}} \\ \text{\frac{\partial u}{\partial t} - \nabla \cdot (\left(u^{m-1} \nabla(-\Delta)^{-\sigma} u)\right)=0,} \\ \text{\end{equation}} \end{array}$$

for  $\sigma \in (0, 1)$ . The model was introduced by Caffarelli and Vázquez in 2011, and is currently one of two main nonlocal extensions of the local porous medium equation. It has finite speed of propagation and comes from a nonlocal Fick's law, but as opposed to the other extension, it does not satisfy the comparison principle. Without comparison, the analysis is difficult. Uniqueness is only known in 1d, where one can exploit that the "cumulative density"  $v(x, t) = \int_{-\infty}^y u(y, t) dy$  satisfies

$$\begin{aligned} \begin{array}{l} \text{\begin{equation}\text{\tag{FPE}}\end{equation}} \\ \text{\frac{\partial v}{\partial t} + \partial_x v^{m-1} (-\Delta)^{\sigma} v = 0, \quad s=1-\sigma,} \\ \text{\end{equation}} \end{array}$$

which is a nonlocal quasilinear parabolic equation in nondivergence form that can be analyzed through viscosity solution methods.

Our numerical method then loosely speaking consists in discretizing this "integrated" equation with a difference quadrature scheme and then compute the solution  $u$  of (FPE) via numerical differentiation. Using upwinding in non-traditional way, we obtain a new type of monotone schemes that allows for convergence analysis via the Barles-Perthame-Souganidis half-relaxed limit method. Combining this result with tightness arguments, we then prove convergence of the approximations of the original problem in the Rubinstein-Kantorovich/Wasserstein-1 distance uniformly in time.

Our results cover both absolutely continuous and Dirac or point mass initial data, and in the latter case, machinery for discontinuous viscosity solutions are needed in the analysis.

00036 (2/3) : 1D @G602 [Chair: David Gómez-Castro]

## [05097] Uniform spectral gap in nonlocal-to-local approximations of diffusion

**Format :** Talk at Waseda University

**Author(s) :** José Cañizo (Universidad de Granada)

**Abstract :** We consider the nonlocal diffusion equation  $\partial_t u = \frac{1}{\epsilon^2} (J_\epsilon * u - u) + \nabla \cdot (xu)$ , where  $J_\epsilon(x) = \epsilon^{-d} J(x/\epsilon)$ , posed for  $t \geq 0$  and  $x \in \mathbb{R}^d$ . This equation approximates the standard Fokker-Planck equation as  $\epsilon \rightarrow 0$ , and serves as a good test ground for several techniques used to study the long-time behaviour of nonlocal PDE. In particular, entropy techniques are not easy to apply here, and lead to functional inequalities which are not well understood. Using probabilistic techniques we show that the above equation has a uniformly positive spectral gap as  $\epsilon \rightarrow 0$ , and we link this to quantitative versions of the central limit theorem. This problem has links to numerical analysis and to some models in mathematical biology, which will also be discussed.

## [03996] Concentration phenomena arising in Aggregation Fast-Diffusion equations

**Format :** Talk at Waseda University

**Author(s) :** Alejandro Fernández-Jiménez (University of Oxford)

**Abstract :** We will discuss about the asymptotic behaviour of the family of Aggregation-Diffusion Equations

$$\partial_t \rho = \Delta \rho^m + \operatorname{div}(\rho \nabla(V + W * \rho)), \quad (1)$$

for \$0

## [05394] Sharp uniform-in-time propagation of chaos on the torus

**Format :** Online Talk on Zoom

**Author(s) :** Rishabh Sunil Gvalani (Max Planck Institute for Mathematics in the Sciences) Matías Delgadino (The University of Texas at Austin)

**Abstract :** We prove uniform-in-time propagation of chaos for weakly interacting diffusions with gradient drift on the torus. Our results are sharp both in terms of the rate (i.e.  $N^{-\frac{1}{2}}$ ) and validity (they hold in the full subcritical range of temperatures). The proof relies on directly controlling the path-space relative entropy between the  $N$  particle system and  $N$  i.i.d copies of the synchronously-coupled limiting McKean SDE. This is joint work with Matias Delgadino.

## [04109] Limiting gradient flow structure of deep linear neural networks

**Format :** Online Talk on Zoom

**Author(s) :** Xavier Fernandez-Real (EPFL)

**Abstract :** We present recent results with L. Chizat, M. Colombo, A. Figalli, on the infinite-width limit of deep linear neural networks initialized with random parameters. We show that, when the number of neurons diverges, the training dynamics converge (in a precise sense) to the dynamics obtained from a gradient descent on an infinitely wide deterministic linear neural network.

00036 (3/3) : 1E @G602 [Chair: José Antonio Carrillo]

## [04224] Deterministic Particle Approximation for aggregation-diffusion equations: entropy solutions, gradient flows, graph.

**Format :** Talk at Waseda University

**Author(s) :** Simone Fagioli (University of L'Aquila)

**Abstract :** We investigate the existence of weak type solutions for a class of aggregation-diffusion PDEs with nonlinear mobility obtained as deterministic large particle limit of a suitable nonlocal versions of the follow-the-leader scheme, which is interpreted as the discrete Lagrangian approximation of the target continuity equation. We prove the well-posedness of entropy solutions for a wide class of nonlocal transport equations with nonlinear mobility in one spatial dimension. At the same time, we expose a rigorous gradient flow structure for this class of equations in terms of an Energy-Dissipation balance, which we obtain via the asymptotic convergence of functionals. The well-posedness is also investigated for aggregation/diffusion equation modeling the evolution of opinion formation on an evolving graph.

## [03893] Non-local PDEs on graphs

**Format :** Online Talk on Zoom

**Author(s) :** André Schlichting (University of Münster)

**Abstract :** This talk reviews some recent results on nonlocal PDEs describing the evolution of a density on discrete graph structures. These structures can arise from applications in the data science field, or they can also be obtained by a numerical discretization of a continuum problem. We also show how those equations are linked to their continuous counterpart in suitable local limits.

## [00037] Recent advances in modelling and simulation of interfacial flows

**Session Time & Room :**

00037 (1/2) : 3D (Aug.23, 15:30-17:10) @D402

00037 (2/2) : 3E (Aug,23, 17:40-19:20) @D402

**Type :** Proposal of Minisymposium

**Abstract :** Interfacial flows arise in numerous natural and technological applications spanning a wide range of length scales from lab-on-a-chip systems to planetary-scale flows. From a purely scientific perspective, these flows pose fundamental theoretical, computational, and experimental challenges to explain complex phenomena including the formation of coherent structures and wave-breaking, as well as phase and topological transitions. Advances in understanding have opened the way for new schemes that allow for precision optimisation and control. This minisymposium will bring together an array of cross-disciplinary specialists, working at the cutting edge of the field, to share their expertise and to exchange ideas.

**Organizer(s) :** Mark Blyth, Anna Kalogirou, Alexander Wray**Classification :** 76-10, 76A20, 76E17**Minisymposium Program :**

00037 (1/2) : 3D @D402 [Chair: Mark Blyth]

## [02292] Interfacial flows and their modelling and control

**Format :** Online Talk on Zoom

**Author(s) :** Alexander Wray (University of Strathclyde)Radu Cimpeanu (University of Warwick)Susana Gomes (University of Warwick)

**Abstract :** Interfacial flows are ubiquitous in nature and industry, and modelling, understanding and controlling them has applications everywhere from carbon sequestration to medical diagnostics. As an introduction to this session, we provide an overview of the topic area, particularly with regards to the state of the art and relevant applications. We also discuss our recent work on controlling the full Navier-Stokes equations using reduced-order models as an example of tying together many of these research strands.

## [05417] New perspectives on continuous film flow over non-planar substrate: a family affair

**Format :** Talk at Waseda University**Author(s) :** Markus Scholle (Heilbronn University )Philip H. Gaskell (Durham University)

**Abstract :** Film flow on curved substrate is investigated theoretically for: (i) continuously-fed, full coverage; (ii) partial coverage following deposition of a fixed liquid volume; (iii) rivulet formation. Using a novel variational formulation uncovers the presence of an interrelated family of flows for 3D axisymmetric geometries and related 2D counterparts. Analytic solutions for local film thickness and the internal flow are obtained, together with rigorous identification of associated timescales, via asymptotic analysis combined with the long-wave approximation.

## [02788] Nonlinear dynamics of unstably stratified two-layer shear flow in a horizontal channel

**Format :** Talk at Waseda University**Author(s) :** Anna Kalogirou (University of Nottingham)Mark Blyth (University of East Anglia)

**Abstract :** The Rayleigh-Taylor instability at the interface of two sheared fluid layers in a horizontal channel is investigated. The dynamics of the flow is described by a nonlinear lubrication equation which is solved numerically for adverse density stratifications, revealing a number of interfacial phenomena including finger-like protrusions, coalescence, saturated travelling waves, and near-segregation of the two fluids. The finer structure of the interface is exposed through asymptotic analysis and is compared to numerical results of the lubrication model as well as direct numerical simulations, displaying an excellent agreement between the three in terms of interfacial structure, wave speed and film thicknesses.

## [04110] Neural network methods for solving interface problems

**Format :** Talk at Waseda University

**Author(s) :** Te-Sheng Lin (National Yang Ming Chiao Tung University)Ming-Chih Lai (National Yang Ming Chiao Tung University, Taiwan)Wei-Fan Hu (National Central University)Yu-Hau Tseng (National University of Kaohsiung)

**Abstract :** Neural networks have emerged as powerful tools for numerically solving partial differential equations. In this talk, we will discuss our recent work using neural network approaches to elliptic interface problems, and possible extensions to deal with models arising from interfacial phenomena. Specifically, we will introduce a structure enforcement layer in the network to enforce the inherent properties of the solutions to given problems, such as discontinuity or periodicity. The structure enforcement layer offers a new approach to solving such problems compared to traditional neural networks, which may struggle to represent discontinuous functions and may not have built-in periodicity.

00037 (2/2) : 3E @D402 [Chair: Anna Kalogirou]

## [05355] On the transition to dripping of an inverted liquid film

**Format :** Talk at Waseda University

**Author(s) :** Mark Blyth (University of East Anglia)Dmitri Tseluiko (Loughborough)Te-Sheng Lin (National Yang Ming Chiao Tung University)

**Abstract :** We discuss the transition to dripping in the gravity-driven motion of a liquid film under an inclined plate. Attention is focused on calculating travelling-wave solutions, for fixed fluid volume and fixed flow rate, using model lubrication equations and the full Stokes equations, and tracking the travelling-wave solution branch as the inclination angle of the plate is increased. Where the branch reaches a turning point we posit that the onset to dripping occurs.

## [03447] Influence of an elastic sheet on impact on a liquid surface

**Format :** Talk at Waseda University

**Author(s) :** Doireann O'Kiely (MACSI, University of Limerick)Finn Box (University of Manchester)Ousmane Kodio (MIT)Dominic Vella (University of Oxford)

**Abstract :** Impact at a liquid-air interface changes when an elastic sheet floats on the liquid surface. A ripple propagates out from the point of impact, but has a wavefront  $r_m \sim t^{1/2}$  rather than the  $r_m \sim t^{2/3}$  typical of capillary waves. We discuss the behaviour of the "elastocapillary ripple", and reduce this new impact problem to a one-parameter similarity problem which interpolates between the limits of a point impactor and Wagner theory.

## [03420] Spin Coating on a Non-Axisymmetric Curved Substrate

**Format :** Talk at Waseda University

**Author(s) :** Ross Geoffrey Shepherd (University of Cambridge)Edouard Boujo (Ecole Polytechnique Federale de Lausanne)Mathieu Sellier (University of Canterbury)

**Abstract :** Spin coating is used to apply functional coatings to flat substrates in the manufacturing of a range of electronic and optical components. Here, we develop a generalised model for the flow of a spin-coated film over an arbitrary substrate geometry, incorporating gravitational, surface tension, centrifugal, and Coriolis forces. In particular, we demonstrate the effects of the Coriolis force on the formation of fingering instabilities and the flow during the early stages of spin coating.

## [05432] Evaporation and the coffee-ring effect for non-circular droplets

**Format :** Online Talk on Zoom

**Author(s) :** Madeleine Moore (University of Hull)Alexander Wray (University of Strathclyde)

**Abstract :** Diffusion-limited evaporation of liquid droplets is commonplace in industrial applications such as microscale patterning and Q/OLED production. However, beyond simple geometries, there are few analytical solutions. Here, we derive asymptotic results for the evaporative flux of a weakly non-circular droplet and demonstrate how these may be used to find the 'coffee ring' for large droplets, with excellent agreement to numerical simulations. Then, we show how the mathematical framework may be extended to polygonal drops.

# [00038] Frontiers of gradient flows: well-posedness, asymptotics, singular limits

**Session Time & Room :**

00038 (1/2) : 1C (Aug.21, 13:20-15:00) @G710

00038 (2/2) : 1D (Aug.21, 15:30-17:10) @G710

**Type :** Proposal of Minisymposium

**Abstract :** Gradient flows, a type of dynamics where systems follow steepest descent paths of various functionals, are ubiquitous in many areas of science and technology. Their mathematical understanding is still developing. Ideas like evolutionary variational inequalities, notions of slope, or very weak definitions originating from dynamical systems allow for far-reaching generalizations. Nonetheless, obstacles such as lack of convexity, non-trivial weights, or complicated geometric settings still cause difficulties. We would like to gather experts within the broad limits we stated, dealing with well-posedness and properties of gradient flows in non-classical cases, as well as singular limits or asymptotics.

**Organizer(s) :** Yoshikazu Giga, Michal Lasica, Piotr Rybka

**Classification :** 35A01, 35A02, 37L05, 35B40, 53E10

**Minisymposium Program :**

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00038 (1/2) : 1C @G710 [Chair: Yoshikazu Giga]

## [05191] Existence for a class of fourth-order quasilinear parabolic systems

**Format :** Talk at Waseda University

**Author(s) :** Michał Łasica (Polish Academy of Sciences)Yoshikazu Giga (the University of Tokyo)

**Abstract :** We consider a class of nonlinear fourth-order parabolic systems of PDEs formally arising as gradient flows of  $p$ -Dirichlet type energies with respect to  $H^{-1}$  metrics weighted by spatial derivatives of the solution up to second order. PDEs with such structure appear for example in modeling of thermal fluctuations in crystal surfaces. We prove global existence of weak solutions. Our tools include a variant of Galerkin scheme, monotonicity methods, and interpolation.

## [03572] Evolutionary limit of gradient flows in heterogeneous Wasserstein space

**Format :** Online Talk on Zoom

**Author(s) :** Yuan Gao (Purdue University)

**Abstract :** The Fokker-Planck equation with fast oscillated coefficients can be regarded as a gradient flow in Wasserstein space with heterogeneous medium. We will use an evolutionary variational approach to obtain the homogenized dynamics, which preserves the gradient flow structure in a limiting homogenized Wasserstein space. Equivalent formulations for heterogeneous Wasserstein distance and their limits will also be discussed.

## [04719] The fourth-order total variation flow in $\mathbf{R}^n$

**Format :** Talk at Waseda University

**Author(s) :** Hirotoshi Kuroda (Hokkaido University)Yoshikazu Giga (the University of Tokyo)Michał Łasica (Polish Academy of Sciences)

**Abstract :** We characterize the solution in terms of what is called the Cahn-Hoffman vector field, and introduce a notion of calibrability of a set in our fourth-order setting.

This notion is related to whether a characteristic function preserves its form throughout the evolution.

If  $n \neq 2$ , all annuli are calibrable.

In the case  $n = 2$ , if an annulus is too thick, it is not calibrable.

## [05426] Global existence for the p-Sobolev flow

**Format :** Online Talk on Zoom

**Author(s) :** Masashi Misawa (Kumamoto University)

**Abstract :** We shall talk about the global existence of the p-Sobolev flow.

The p-Sobolev flow is regarded as the heat flow associated with the Sobolev inequality and the nonlinear eigenvalue problem corresponding to it. We shall study the asymptotic behavior of the p-Sobolev flow and present the so-called volume concentration phenomenon at time-infinity.

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00038 (2/2) : 1D @G710 [Chair: Piotr Rybka]

## [02587] Weak solutions to gradient flows in metric measure spaces

**Format :** Talk at Waseda University

**Author(s) :** Jose M Mazon (Universitat de Valencia)

**Abstract :** We show how to introduce the notion of weak solutions in metric measure spaces in the model case of the  $p$ -Laplacian evolution equation, including the borderline case  $p = 1$ , i.e., the total variation flow. For  $p > 1$ , it has been previously studied as the gradient flow in  $L^2$  of the  $p$ -Cheeger energy. Using the first-order differential structure on a metric measure space introduced by Gigli, we characterise the subdifferential in  $L^2$  of the  $p$ -Cheeger energy. This leads to a new definition of solutions to the  $p$ -Laplacian evolution equation in metric measure spaces, in which the gradient is replaced by a vector field, defined via Gigli's differential structure, satisfying some compatibility conditions.

## [04233] Duality methods for gradient flows of linear growth functionals

**Format :** Online Talk on Zoom

**Author(s) :** Wojciech Górný (University of Vienna; University of Warsaw)Jose M Mazón (University of València)

**Abstract :** We study gradient flows in  $L^2$  of general convex and lower semicontinuous functionals with linear growth. Typical examples of such evolution equations are the time-dependent minimal surface equation and the total variation flow. Classical results concerning characterisation of solutions require a special form or differentiability of the

Lagrangian; we apply a duality-based method to formulate a general definition of solutions, prove their existence and uniqueness, and reduce the regularity and structure assumptions on the Lagrangian.

### [04556] Convergence of Sobolev gradient trajectories to elastica

**Format :** Talk at Waseda University

**Author(s) :** Shinya Okabe (Tohoku University)

**Abstract :** In this talk we consider the  $H^2(ds)$ -gradient flow for the modified elastic energy defined on closed immersed curves in  $\mathbb{R}^n$ . We prove (i) the existence of a unique global-in-time solution to the flow; (ii) the full limit convergence of solutions to elastica without any additional reparametrization and translation. The main ingredients of the proof of (ii) are a Lojasiewicz-Simon's gradient inequality and the completeness of a  $H^2(ds)$ -Riemannian metric space.

### [05251] Recent advances in Sobolev gradient flows of plane curves

**Format :** Talk at Waseda University

**Author(s) :** Glen Wheeler (University of Wollongong)

**Abstract :** In this talk, we discuss recent progress made alongside Shinya Okabe, Philip Schrader, and Valentina-Mira Wheeler in studying the relationship between the classical curve shortening flow and the triviality of the  $L^2(ds)$  metric. Our method is to study gradient flows with different metrics (that give rise to non-trivial metric spaces). Our investigation with global analysis reveals intriguing behavior.

## [00047] Combining Machine Learning and Stochastic Methods for Modeling and Forecasting Complex Systems

**Session Time & Room :**

00047 (1/3) : 3E (Aug.23, 17:40-19:20) @E804

00047 (2/3) : 4C (Aug.24, 13:20-15:00) @E804

00047 (3/3) : 4D (Aug.24, 15:30-17:10) @E804

**Type :** Proposal of Minisymposium

**Abstract :** Complex Systems are ubiquitous in different areas. Recent development of advanced machine learning tools and new stochastic modeling strategies introduce new insights and approaches of advancing the study of complex systems. This minisymposium aims at combining data-driven and physics-based methods to improve the current understanding, modeling and forecasting methods of various complex systems containing different features. Topics of this minisymposium include, but are not limited to, physics-driven machine learning techniques, efficient stochastic multiscale modeling approaches, data assimilation, uncertainty quantification, inverse problems, statistical control, surrogate and reduced order models as well as efficient forecast algorithms.

**Organizer(s) :** Nan Chen, Di Qi

**Classification :** 68T09, 35R60, 76F55, 60H30, 37N10

**Minisymposium Program :**

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00047 (1/3) : 3E @E804 [Chair: Di Qi]

### [03378] Generative modelling through diffusion maps

**Format :** Talk at Waseda University

**Author(s) :** Georg A. Gottwald (University of Sydney)Sebastian Reich (Universität Potsdam)Fengyi Li (MIT)

**Abstract :** We propose a Langevin sampler as a generative modelling method. The Langevin sampler is constructed using diffusion maps. We show how this method can be used to perform inverse modelling tasks as well as providing a stochastic subgrid-scale parametrisation.

## [04604] Tracer Prediction in Simplified Stochastic Geophysical Models through Kalman Filters and Related Methods

**Format :** Talk at Waseda University

**Author(s) :** Mustafa A Mohamad (University of Calgary)

**Abstract :** Transport-dominated phenomena represents a major challenge for reduction techniques due to the presence of nonlinear coherent wave structures. Here we discuss the assimilation and prediction of a turbulent complex flow field given a stream of measurements provided by passively advected Lagrangian drifters. We quantify recovery of the Eulerian energy spectra from observations of Lagrangian drifters by special data assimilation algorithms. We primarily focus on algorithms based on Kalman filters, but also discuss related methods for comparison. The focus is on statistical properties of the tracer.

## [05043] Machine Learning for Stochastic Parametrisation

**Format :** Online Talk on Zoom

**Author(s) :** Hannah Christensen (University of Oxford)

**Abstract :** The use of stochastic techniques in atmospheric models to characterise uncertainty in small-scale processes has proved beneficial for forecasts on weather, seasonal and climate timescales. We have also recently seen significant progress in replacing the parametrisation schemes which represent these small-scale processes using machine learning (ML). This has the potential to speed up and improve numerical models. In this presentation I bring together these two developments, and discuss approaches to use ML for stochastic parametrisation.

## [03280] Explainable AI to Detect, Predict and Discover Climate Variability and Change

**Format :** Online Talk on Zoom

**Author(s) :** Elizabeth Barnes (Colorado State University)

**Abstract :** Earth's climate is chaotic and noisy. Finding usable signals amidst all of the noise can be challenging: be it predicting if it will rain, knowing which direction a hurricane will go, understanding the implications of melting Arctic ice, or detecting the impacts of human-induced climate warming. Here, I will demonstrate how explainable artificial intelligence (XAI) techniques can sift through vast amounts of climate data and push the bounds of scientific discovery: allowing scientists to ask "why?" but now with the power of machine learning.

00047 (2/3) : 4C @E804 [Chair: Nan Chen]

## [05245] semi-supervised active learning on graphs

**Format :** Online Talk on Zoom

**Author(s) :** Andrea Bertozzi (UCLA)

**Abstract :** Similarity graphs are a popular technique for semi-supervised machine learning. They have an advantage over more modern neural network methods in that they can perform well with a modest amount of training data. I will present an active learning framework in which additional training data is introduced through a human in the loop. This approach can outperform prior state of the art on several remote sensing problems such as object recognition in synthetic aperture radar and multispectral and hyperspectral imagery.

## [04307] Integrating the spectral analyses of neural networks and nonlinear physics for explainability, generalizability, and stability

**Format :** Talk at Waseda University

**Author(s) :** Pedram Hassanzadeh (Rice U)Ashesh Chattopadhyay (PARC)Yifei Guan (Rice U)Adam Subel (NYU)

**Abstract :** I will introduce a new framework that combines the spectral (Fourier) analyses of NNs and nonlinear physics, and leverages recent advances in theory and applications of deep learning, to move toward rigorous analysis of deep NNs for applications involving dynamical systems. I will use examples from subgrid-scale modeling of 2D turbulence and Rayleigh-Bernard turbulence and forecasting extreme weather to show how this framework can be used to systematically address challenges about explainability, generalizability, and stability.

## [03737] Shock trace prediction by reduced models for a viscous stochastic Burgers equation

**Format :** Talk at Waseda University

**Author(s) :** Fei Lu (Johns Hopkins University)

**Abstract :** Can data-driven reduced models predict extreme events in nonlinear multiscale systems? Using stochastic Burgers equation's random shocks as a prototype of extreme events, we demonstrate that although large-scale dominating dynamics-focused reduced models cannot represent shocks, they can accurately predict shock trace—the timing and locations of shocks—with relatively low false prediction rates. The data-driven closure terms are critical in capturing unresolved small-scale dynamics' effects on resolved ones.

## [01386] A Multi-Fidelity Ensemble Kalman Filter with Adaptive Reduced-Order Models

**Author(s) :** Francesco Attilio Bruno Silva (Eindhoven University of Technology) Cecilia Pagliantini (Eindhoven University of Technology) Karen Veroy (Eindhoven University of Technology)

**Abstract :** Recently there has been an increased interest in combining model order reduction techniques and ensemble-based methods for state estimation of complex systems. Data assimilation algorithms have been proposed to jointly use low and high-fidelity ensembles, e.g., the MFEKF. The construction of low-fidelity models in the offline stage, however, leads these methods into a trade-off between accuracy and computational costs. In our research, we developed adaptive reduced-basis techniques with online modified approximation spaces to mitigate this issue.

00047 (3/3) : 4D @E804 [Chair: Mustafa Mohamad]

## [05228] Embedding classical dynamics in a quantum computer

**Format :** Online Talk on Zoom

**Author(s) :** Dimitrios Giannakis (Dartmouth College)

**Abstract :** We present a framework for simulating classical dynamical systems by quantum systems running on a quantum computer. The framework employs a quantum feature map for representing classical states by density operators on a reproducing kernel Hilbert space,  $\mathcal{H}$ . Simultaneously, a mapping is employed from classical observables into self-adjoint operators on  $\mathcal{H}$  such that quantum expectation values are consistent with pointwise function evaluation. We illustrate our approach with quantum circuit simulations and experiments on quantum computers.

## [05225] Machine learning correction operators for capturing extremes in coarse scale climate models

**Format :** Online Talk on Zoom

**Author(s) :** Themistoklis Sapsis (MIT)

**Abstract :** This work presents a systematic framework for improving the predictions of statistical quantities for turbulent systems, with a focus on correcting coarse climate simulations. We also provide quantification measures for the value of data towards this goal. Machine learning correction operators for chaotic systems is challenging as learning errors due to chaotic divergence is not meaningful. The presented approach combines dynamical systems and probabilistic data-driven ideas. We apply the framework to E3SM climate simulations.

## [04015] A Framework for Machine Learning of Model Error in Dynamical Systems

**Format :** Talk at Waseda University

**Author(s) :** Matthew Levine (Caltech) Andrew Stuart (Caltech)

**Abstract :** The development of data-informed predictive models for dynamical systems is of widespread interest in many disciplines. Here, we present a unifying framework for blending mechanistic and machine-learning approaches for identifying dynamical systems from data. This framework is agnostic to the chosen machine learning model parameterization, and casts the problem in both continuous- and discrete-time. We will also show recent developments that allow these methods to learn from noisy, partial observations. We first study model error from the learning theory perspective, defining the excess risk and generalization error. For a linear model of the error used to learn about ergodic dynamical systems, both excess risk and generalization error are bounded by terms that diminish with the square-root of T (the length of the training trajectory data). In our numerical examples, we first study an idealized, fully-observed Lorenz system with model error, and demonstrate that hybrid methods substantially outperform solely data-driven and solely mechanistic-approaches. Then, we present recent results for modeling partially observed Lorenz dynamics that leverages both data assimilation and neural differential equations. Joint work with Andrew Stuart.

## [05032] Combining physical and machine learning forecasts for Earth system prediction

**Format :** Talk at Waseda University

**Author(s) :** Eviatar Bach (California Institute of Technology)

**Abstract :** Machine learning (ML) holds the potential to improve Earth system prediction by learning directly from data, bypassing deficiencies in existing dynamical models. Hybrid methods, which combine ML with dynamical models, leverage the strengths of both approaches. I will present two hybrid methods that use tools from data assimilation: Ensemble Oscillation Correction, a forecasting method for combining ML forecasts of specific modes with a full-field dynamical model, and the Multi-Model Ensemble Kalman Filter, a more general method for integrating multiple forecast models with observations.

## [00048] Interfaces between kinetic equations and many-agent social systems. Part I

**Session Time & Room :**

00048 (1/3) : 2C (Aug.22, 13:20-15:00) @G702

00048 (2/3) : 2D (Aug.22, 15:30-17:10) @G702

00048 (3/3) : 2E (Aug.22, 17:40-19:20) @G702

**Type :** Proposal of Minisymposium

**Abstract :** In recent years, kinetic-type models emerged to be a powerful mathematical framework for the description of emerging patterns in systems composed by a large number of agents. Furthermore, the natural multiscale nature of these equations, linking microscopic unobservable social forces to macroscopic measurable patterns, permits an efficient investigation of collective phenomena in a heterogeneity of disciplines, like biology, social sciences and robotics. In this minisymposium we collect novel perspectives from experts actively working on these research problems.

**Organizer(s) :** Giacomo Dimarco, Young-Pil Choi

**Classification :** 35Q20, 35Q84, 35Q91, 35Q92, 49N80

**Minisymposium Program :**

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00048 (1/3) : 2C @G702 [Chair: Mattia Zanella]

## [03361] Multi Agent System for Inverse Problems

**Format :** Talk at Waseda University

**Author(s) :** Michael Herty (RWTH Aachen University)

**Abstract :** We are interested in the construction of numerical methods for constrained high-dimensional constrained nonlinear optimization problems by gradient free techniques. Gradients are replaced by particle approximations and recently different methods have been proposed, e.g. consensus-based, swarm-based or ensemble Kalman based methods. We discuss recent extensions to the constrained and the parametric case as well as their corresponding mean field descriptions in the many particle limit. Those allow to show convergence as well as the analysis of properties of the new algorithm. Several numerical examples, also in high dimensions, illustrate the theoretical findings as well as the performance of those methods.

## [03822] Parameter estimation for macroscopic pedestrian dynamics models using microscopic data

**Format :** Talk at Waseda University

**Author(s) :** Susana Gomes (University of Warwick)

**Abstract :** I will present a framework for estimating relevant parameters for pedestrian dynamics by fitting a macroscopic model for crowd dynamics using data from pedestrian trajectories. The model couples a density dependent stochastic differential equation, to a nonlinear partial differential equation for the density via the fundamental diagram. I will discuss identifiability of the parameters, introduce optimisation and Bayesian methods to perform the identification, and analyse the performance of the proposed methodology in various realistic situations.

## [03518] Navigation system based routing strategies in traffic flows on networks

**Format :** Talk at Waseda University

**Author(s) :** Adriano Festa (Politecnico di Torino)

**Abstract :** Navigation choices play an important role in modeling and forecasting traffic flows on road networks. We introduce a macroscopic differential model coupling a conservation law with a Hamilton-Jacobi equation to respectively model the nonlinear transportation process and the strategic choices of users. Furthermore, the model is adapted to the multi-population case, where every population differs in the level of traffic information about the system.

## [02357] Uncertainty quantification in vehicular traffic models

**Format :** Talk at Waseda University

**Author(s) :** Elisa Iacomini (University of Ferrara, Department of Mathematics and Computer Science)

**Abstract :** Traffic models have been widely studied, however limitations for obtaining reliable forecasts are still present. Recently it has been pointed out how traffic is exposed to the presence of uncertainties. In this talk, starting from the hierarchy between microscopic, kinetic and macroscopic scales, we will investigate the propagation of uncertainties through the models. Connections between the scales will be presented in the stochastic scenario and numerical simulations will be performed.

00048 (2/3) : 2D @G702 [Chair: Giacomo Dimarco]

## [04654] On a kinetic Elo rating model for players with dynamical strength

**Format :** Talk at Waseda University

**Author(s) :** Bertram Düring (University of Warwick)

**Abstract :** We discuss a new kinetic rating model for a large number of players, which is motivated by the well-known Elo rating system. Each player is characterised by an intrinsic strength and a rating, which are both updated after each game. We state and analyse the respective Boltzmann-type equation and derive the corresponding nonlinear, nonlocal Fokker-Planck equation. We investigate the existence of solutions to the Fokker-Planck equation and discuss their behaviour in the long time limit. Furthermore, we illustrate the dynamics of the Boltzmann and Fokker-Planck equation with various numerical experiments.

## [04235] Nonlocal approximation of nonlinear diffusion equations and cross-diffusion systems

**Format :** Talk at Waseda University

**Author(s) :** Antonio Esposito (University of Oxford) Martin Burger (University of Hamburg) José Antonio Carrillo (University of Oxford) Jeremy S.-H. Wu (UCLA)

**Abstract :** In this talk I will discuss the connection between a class of nonlocal PDEs and nonlinear diffusion equations, including porous medium PDEs and cross-diffusion systems. As byproduct of this link, one can obtain a rigorous deterministic particle approximation for the PDEs considered. The analysis is based on a suitable regularisation of the associated free energy using gradient flow techniques. However, the strategy proposed relies on a discretisation scheme, so-called JKO, which can be slightly modified in order to extend the results to PDEs without gradient flow structure. In particular, it does not require convexity of the associated energies. The talk is based on two joint works with M. Burger (FAU Erlangen-Nuremberg), and J. A. Carrillo (Oxford) and J. Wu (UCLA).

## [04374] Kinetic models for multi-agent systems with multiple microscopic states

**Format :** Talk at Waseda University

**Author(s) :** Nadia Loy (Politecnico di Torino)

**Abstract :** In this talk we present a class of kinetic models describing interactions among individuals having multiple microscopic states. We shall consider microscopic states evolving according to both stochastic dependent and independent processes. In particular, we shall consider interacting agents who are divided into multiple sub-populations. As such, the agents are not indistinguishable, as classically assumed in kinetic theory, within the whole population. A general framework allowing to describe binary interactions and transfers among different sub-groups by deriving the model from microscopic stochastic processes will be presented. We shall discuss formal results concerning existence, uniqueness and equilibria. Moreover, we shall illustrate applications to wealth exchange models with migration.

## [03362] Modelling coevolutionary dynamics in heterogeneous SI epidemiological systems across scales

**Format :** Talk at Waseda University

**Author(s) :** Elisa Paparelli (Politecnico di Torino) Tommaso Lorenzi (Politecnico di Torino) Andrea Tosin (Politecnico di Torino)

**Abstract :** We present a new structured compartmental epidemiological model for the coevolutionary dynamics between susceptible and infectious individuals. Specifically, continuous structuring variables capture interindividual variability in resistance to infection and viral load. The model comprises a system of integro-differential equations providing a Boltzmann-type kinetic description of corresponding stochastic particle dynamics. We discuss a formal derivation of this model from the underlying particle dynamics and present analytical and numerical results on the long-time behaviour of its solutions.

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00048 (3/3) : 2E @G702 [Chair: Giacomo Dimarco]

## [05559] The Collisional Particle-In-Cell Method for the Vlasov-Maxwell-Landau System

**Format :** Talk at Waseda University

**Author(s) :** Rafael Bailo (University of Oxford, Mathematical Institute) José Antonio Carrillo (University of Oxford, Mathematical Institute) Jingwei Hu (University of Washington)

**Abstract :** In this talk we will present an extension of the classical Particle-In-Cell (PIC) method for plasmas which can account for the collisional effects modelled by the Landau operator. The method is derived from the gradient-flow formulation of the Landau equation, thereby preserving the collision invariants and the entropy structure. We will discuss the derivation and implementation of the method, as well as several numerical examples to showcase the effects of collisions in plasma simulations.

## [00049] Interfaces between kinetic equations and many-agent social systems. Part II

**Session Time & Room :**

00049 (1/3) : 3C (Aug.23, 13:20-15:00) @G702

00049 (2/3) : 3D (Aug.23, 15:30-17:10) @G702

00049 (3/3) : 3E (Aug.23, 17:40-19:20) @G702

**Type :** Proposal of Minisymposium

**Abstract :** In recent years, kinetic-type models emerged to be a powerful mathematical framework for the description of emerging patterns in systems composed by a large number of agents. Furthermore, the natural multiscale nature of these equations, linking microscopic unobservable social forces to macroscopic measurable patterns, permits an efficient investigation of collective phenomena in a heterogeneity of disciplines, like biology, social sciences and robotics. In this minisymposium we collect novel perspectives from experts actively working on these research problems.

**Organizer(s) :** Giacomo Dimarco, Young-Pil Choi, Mattia Zanella

**Classification :** 35Q20, 35Q84, 35Q91, 35Q92, 49N80

**Minisymposium Program :**

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00049 (1/3) : 3C @G702 [Chair: Young-Pil Choi]

## [04948] Weak couplings of Lohe type aggregation models

**Format :** Online Talk on Zoom

**Author(s) :** Seung Yeal Ha (Seoul National University) Dohyun Kim (Sungkyunkwan University) Hansol Park (Simon Fraser University)

**Abstract :** In this talk, we present a systematic algebraic approach for the weak coupling of Cauchy problems to multiple Lohe tensor models. For this, we identify an admissible Cauchy problem to the Lohe tensor (LT) model with a characteristic symbol consisting of four tuples in terms of a size vector, a natural frequency tensor, a coupling strength tensor and admissible initial configuration. In this way, the collection of all admissible Cauchy problems to the LT models is equivalent to the space of characteristic symbols. On the other hand, we introduce a binary operation, namely

part\_1

fusion operation" as a binary operation between characteristic symbols. It turns out that the fusion operation satisfies an associativity and admits the identity element in the space of characteristic symbols which naturally forms a monoid. By virtue of the fusion operation, the weakly coupled system of multi tensor models can be obtained by applying the fusion operation of multiple characteristic symbols corresponding to the Lohe tensor models. As a concrete example, we consider a weak coupling of the swarm sphere model and the Lohe matrix model, and provide sufficient framework leading to emergent dynamics to the proposed weakly coupled model. This is a joint work with Dohyun Kim (Sungshin Women's Univ.) and Hansol Park (Simon Fraser Univ.)

## [03897] Quantified overdamped limit for Kinetic Vlasov-Fokker-Planck equations

**Format :** Talk at Waseda University

**Author(s) :** Oliver Tse (Eindhoven University of Technology)Young-Pil Choi (Yonsei University)

**Abstract :** The study of the overdamped limit for the kinetic Fokker-Planck equation has been of interest since the seminal work of Kramers in 1940, where he formally discussed the convergence by introducing a coarse-graining map. This talk is based on work with Young-Pil Choi, where we provide a framework to establish quantitative estimates for the overdamped limit of the kinetic Vlasov-Fokker-Planck with singular interaction in terms of the 2-Wasserstein distance.

## [04724] Phase-coupled models for synchronization with nonlocal temporal interactions

**Format :** Talk at Waseda University

**Author(s) :** Myeongju Kang (Korea Institute for Advanced Study)

**Abstract :** We study the emergent dynamics and global well-posedness of the Kuramoto model with memory effect, which is a system of Volterra-type integro-differential equations on unit circle. We adopt nonlocal temporal interactions to design synchronized behavior of oscillators affected by memories of the past. We first establish the global well-posedness of the Kuramoto model with memory effect, and provide sufficient frameworks for uniform boundedness of the phase diameter. Then, we define an energy functional whose boundedness is guaranteed by the boundedness of the phase diameter. We show that energy functional is monotonically decreasing, which implies complete frequency synchronization. Moreover, when natural frequencies are all identical we show the emergence of complete phase synchronization.

## [04208] Rigorous derivation of the Euler-Alignment model with singular communication weights from a kinetic Fokker-Planck-Alignment model

**Format :** Online Talk on Zoom

**Author(s) :** Young-Pil Choi (Yonsei University)Jeongho Kim (Kyung Hee University)

**Abstract :** We present a rigorous derivation of the isothermal Euler-alignment model with singular communication weights. We consider a hydrodynamic limit of a kinetic Fokker-Planck-alignment model, which is the nonlinear Fokker-Planck equation with the Cucker-Smale alignment force. Our analysis is based on the estimate of relative entropy between macroscopic quantities, together with careful analysis on the singular communication weights.

00049 (2/3) : 3D @G702 [Chair: Giacomo Dimarco]

## [04945] Sticky-particle Cucker-Smale dynamics and the entropic selection principle for the Euler-alignment system

**Format :** Talk at Waseda University

**Author(s) :** Trevor Leslie (University of Southern California)Changhui Tan (University of South Carolina)

**Abstract :** In this talk, I will discuss weak solutions to the Euler-alignment system for collective behaviors. I will introduce an entropic selection principle that serves to isolate a unique weak solution. Notably, the solution can be constructed and approximated using Cucker-Smale dynamics, with sticky particle collision rules. I will present an analytical convergence result, as well as the formation of finite and infinite time clusters.

## [04190] Structure-preserving particle method for the Vlasov-Landau-Maxwell system

**Format :** Online Talk on Zoom

**Author(s) :** Rafa Bailo (University of Oxford)Jose Carrillo (University of Oxford)Jingwei Hu (University of Washington)

**Abstract :** Vlasov-Landau-Maxwell equation is often considered as the first-principle physics model for plasmas. We introduce a novel particle method for this equation which preserves the basic physical properties such as conservation of mass, momentum, and energy, and even decay of entropy. The method is based on a proper regularization of the Landau collision operator so that it can be naturally coupled with the classical particle-in-cell (PIC) method to preserve the part\_1

structure. Various plasma benchmark tests such as collisional Landau damping and two-stream instability will be presented.

## [03372] On solutions to the kinetic Cucker-Smale model with singular communication weights

**Format :** Talk at Waseda University

**Author(s) :** Jinwook Jung (Jeonbuk National University) Young-Pil Choi (Yonsei University)

**Abstract :** In this talk, we investigate the existence of solutions to the kinetic Cucker-Smale model with singular communication weights  $\phi(r) = r^{-\gamma}$ . First, we establish the local-in-time well-posedness of strong solutions to the equation in a weighted Sobolev space for  $\gamma \in [d-1, d+1/4) \setminus \{d\}$ . Secondly, we present the existence of weak solutions for  $\gamma \in [d-1, d)$  and also the uniqueness result when  $\gamma = d-1$ . This talk is based on the collaboration with Y.-P. Choi.

## [03940] Interaction energy minimizers on bounded domains

**Format :** Online Talk on Zoom

**Author(s) :** Ruiwen Shu (University of Georgia) José Carrillo (University of Oxford)

**Abstract :** I will discuss the behavior of interaction energy minimizers on bounded domains. When the interaction potential is more singular than Newtonian, then mass does not tend to concentrate on the boundary; when it is Newtonian or less singular, then mass necessarily concentrate on the boundary for purely repulsive potentials. We also draw a connection between bounded-domain minimizers and whole-space minimizers.

00049 (3/3) : 3E @G702 [Chair: Mattia Zanella]

## [03933] Analytical approaches to the problem of emergence arising in systems of collective behavior

**Format :** Online Talk on Zoom

**Author(s) :** Roman Shvydkoy (University of Illinois at Chicago)

**Abstract :** Emergence is a phenomenon of formation of collective outcomes in systems where communications between agents has local range. For a wide range of applications, such as swarming behavior of animals or exchange of opinions between individuals, such outcomes result in a globally aligned state or congregation of aligned clusters. The classical result of Cucker and Smale states that alignment is unconditional in flocks that have global communication with non-integrable radial tails. Proving a similar statement for purely local interactions is a challenging mathematical problem. In this talk we will overview three programs of research directed on understanding the emergent phenomena: statistical approach to generic alignment for agent-based systems, kinetic approach based on relaxation and hypocoercivity, and hydrodynamic models incorporating a novel way of interaction based on topological communication.

## [00052] Efficient numerical methods for high-dimensional PDEs

**Session Time & Room :**

00052 (1/2) : 1C (Aug.21, 13:20-15:00) @E705

00052 (2/2) : 1D (Aug.21, 15:30-17:10) @E705

**Type :** Proposal of Minisymposium

**Abstract :** Many problems in science and engineering are described by high-dimensional PDEs. Over the years, different numerical techniques have been developed for these problems, including low rank method, sparse grid, tensor method, reduced order modeling, machine learning, optimization, and quantum algorithms, to name a few. In this minisymposium, we bring researchers from a wide spectrum of application areas, such as plasma physics, quantum dynamics, biology, etc. to address the common theme of solving high-dimensional PDEs and exchange ideas.

**Organizer(s) :** Lukas Einkemmer, Jingwei Hu

**Classification :** 65Mxx

**Minisymposium Program :**

00052 (1/2) : 1C @E705 [Chair: Jingwei Hu]

## [04856] Sparse grid techniques for particle-in-cell simulation of kinetic plasmas

**Format :** Online Talk on Zoom

**Author(s) :** Lee Forrest Ricketson (Lawrence Livermore National Laboratory)

**Abstract :** The Vlasov equation, which models collisionless plasma dynamics, is six-dimensional in general. To combat this high dimensionality, the most prevalent numerical method has long been particle-in-cell (PIC), in which the plasma is represented by particles which interact with electromagnetic fields specified on a spatial mesh. However, the inclusion of particles subjects the scheme to slow-converging sampling errors, while use of a spatial mesh admits only partial mitigation of the curse of dimensionality. We show that using sparse grids with PIC makes the algorithm's complexity only logarithmically dependent on dimension and dramatically reduces the impact of sampling noise. We report recent progress combining sparse PIC advanced symplectic and implicit methods. Finally, we report on ongoing work toward adaptively choosing suitable coordinates for these sparse grid computations.

\*Prepared by LLNL under Contract DE-AC52-07NA27344.

## [03639] Nonlinear model reduction with adaptive bases and adaptive sampling

**Format :** Online Talk on Zoom

**Author(s) :** Benjamin Peherstorfer (Courant Institute of Mathematical Sciences, New York University)

**Abstract :** We introduce an online-adaptive model reduction approach that can efficiently reduce convection-dominated problems. It exploits that manifolds are low dimensional in a local sense in time and iteratively learns and adapts reduced spaces from randomly sampled data of the full models to locally approximate the solution manifolds. Numerical experiments to predict pressure waves in combustion dynamics demonstrate that our approach achieves significant speedups in contrast to classical, static reduced models.

## [04871] Quantum Algorithms for Accelerating the Solution of Partial Differential Equations

**Format :** Online Talk on Zoom

**Author(s) :** Ilon Joseph (Lawrence Livermore National Laboratory)

**Abstract :** Quantum algorithms have been proposed to accelerate the solution of linear partial differential equations (PDEs) with polynomial to exponential speedup. Recent progress has significantly improved these algorithms with respect to numerical methods and error convergence. Due to the “no-cloning” theorem, solving nonlinear PDEs is more challenging. Newly proposed Koopman and Carleman approaches solve for the linear evolution of the probability distribution function of the solution and are closely related to simulating stochastic PDEs and quantum fields.

## [03854] A Hybrid AMR Low-Rank Tensor Approach for Solving the Boltzmann Equation

**Format :** Talk at Waseda University

**Author(s) :** William Tsubasa Taitano (Los Alamos National Laboratory) Samuel Jun Araki (Air Force Research Laboratory)

**Abstract :** The Boltzmann equation describes the time evolution of a particle distribution function in a six-dimensional position-velocity phase space. The exponential growth in computational complexity often challenges a grid-based approach to modeling the Boltzmann equation as the dimensionality grows. Scalable low-rank tensor decomposition techniques have recently been developed with applications to high-dimension PDEs to address this issue. Despite the remarkable progress made in the community, low-rank structures in the phase-space are not evident in realistic engineering systems with complex geometries (e.g., electric propulsion systems and fusion reactors), where discontinuities, shocks, complex boundary conditions, and material-dependent physics (e.g., collisions, fusion reactions, ionization/excitation, charge-exchange processes) pose formidable challenges. In this talk, we propose a novel hybrid algorithm where quad-tree adaptive mesh refinement (AMR) is applied in real space while a low-rank approximation is applied in the velocity space. The AMR algorithm efficiently handles challenges pertaining to complex structures in real space, while the low-rank formulation targets dimensionality challenges in the velocity space. We present preliminary results on the new algorithm applied to challenging multi-dimensional gas kinetics problems.

## [04128] Designing High-Dimensional Closed-Loop Optimal Control Using Deep Neural Networks

**Format :** Talk at Waseda University

**Author(s) :** Jiequn Han (Flatiron Institute, Simons Foundation)

**Abstract :** Designing closed-loop optimal control for high-dimensional nonlinear systems remains a long-standing challenge. Traditional methods, such as solving the Hamilton-Jacobi-Bellman equation, suffer from the curse of dimensionality. Recent studies introduced a promising supervised learning approach, utilizing deep neural networks to learn from open-loop optimal control solutions. From a PDE standpoint, this method learns solutions along characteristic lines.

This talk will first overview this method and identify a limitation in its basic form, the distribution mismatch phenomenon, caused by controlled dynamics. We then propose the initial value problem enhanced sampling method to address this issue. The proposed method presents theoretical guarantees of improvement over the basic version in the classical linear-quadratic regulator and demonstrates significant improvement numerically on several high-dimensional nonlinear problems.

## [04563] An Inverse Problem in Mean Field Games from Partial Boundary Measurement

**Format :** Talk at Waseda University

**Author(s) :** Yat Tin Chow (University of California, Riverside)Samy Wu Fung (Colorado School of Mines)Siting Liu (University of California, Los Angeles)Levon Nurbekyan (University of California, Los Angeles)Stanley Osher (University of California, Los Angeles)

**Abstract :** In this talk, we consider a novel inverse problem in mean-field games (MFG). We aim to recover the MFG model parameters that govern the underlying interactions among the population based on a limited set of noisy partial observations of the population dynamics under the limited aperture. Due to its severe ill-posedness, obtaining a good quality reconstruction is very difficult. Nonetheless, it is vital to recovering the model parameters stably and efficiently to uncover the underlying causes of population dynamics for practical needs.

Our work focuses on the simultaneous recovery of running cost and interaction energy in the MFG equations from a finite number of boundary measurements of population profile and boundary movement. To achieve this goal, we formalize the inverse problem as a constrained optimization problem of a least squares residual functional under suitable norms. We then develop a fast and robust operator splitting algorithm to solve the optimization using techniques including harmonic extensions, three-operator splitting scheme, and primal-dual hybrid gradient method. Numerical experiments illustrate the effectiveness and robustness of the algorithm.

## [04470] Automatic partitioning for Boolean CME Low-Rank integrator

**Format :** Talk at Waseda University

**Author(s) :** Martina Prugger (University of Innsbruck)Lukas Einkemmer (University of Innsbruck)

**Abstract :** Cell signaling processes are usually modeled by chemical reactions encoded in a system of ordinary differential equations. The resulting model is deterministic and omits the inherent stochasticity of cell reactions. This is mostly due to the fact, that solving the Chemical Master Equation (CME), which resolves the inherent probabilistic states of the chemical system suffers from the curse of dimensionality. This results in high computational and memory requirements, that prohibit the simulation of the CME for system sizes that are usually required for practical applications.

We developed a low-rank integrator for the CME for Boolean networks that enables us to simulate systems to a size of up to 41 different chemical species on a workstation. An integral part of this method is to partition the network into multiple sub-partitions, on which the CME is solved exactly. Key to an efficient solver is the distribution of species, while keeping the approximation error between the networks to a minimum. While for small networks, this can still be done easily by a person, for a network of the size of e.g., 41 species, this is no longer feasible. We therefore introduce an automatic partitioner by using the Kernighan-Lin algorithm to select multiple networks that minimize the amount of connections between the sub-networks. We then use information entropy that evaluates each of the chosen networks. This results in an automatic partitioning tool that reduces the rank that is required to faithfully resolve the biological dynamics.

# [00057] Many-agent systems and mean-field models for socio-economic and life sciences dynamics

**Session Time & Room :**

00057 (1/2) : 4C (Aug.24, 13:20-15:00) @G702

00057 (2/2) : 4D (Aug.24, 15:30-17:10) @G702

**Type :** Proposal of Minisymposium

**Abstract :** Complex, real-life systems in sociology, economics, and life sciences often consist of a large number of individuals. Through interactions among these individuals a collective behaviour may emerge over time and certain patterns may develop. Examples include pedestrian, evacuation and traffic models, opinion formation, wealth distribution, chemotaxis and flocking/swarming. The aim of the mini-symposium is to highlight recent advances in modelling, analysis, numerics and optimal control of kinetic and PDE models in this area.

**Organizer(s) :** Marie-Therese Wolfram, Bertram Düring

**Classification :** 35Q20, 35Q84, 35Q91, 35Q92

**Minisymposium Program :**

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00057 (1/2) : 4C @G702 [Chair: Bertram Düring]

## [04044] Data-driven kinetic model for opinion dynamics and contacts

**Format :** Talk at Waseda University

**Author(s) :** Giacomo Dimarco (University of Ferrara, Department of Mathematics and Computer Science)

**Abstract :** Opinion dynamics is an important area of research that studies how individuals form and change their opinions in a social context. Understanding the mechanisms that drive opinion formation and change is essential for predicting social phenomena, such as political polarization and the spread of misinformation. In this talk, we present a new model for opinion dynamics in presence of social media contacts, using real-life data from Twitter in order to retrieve the parameters appearing in our model so to make it as close as possible to what happens in reality.

## [02360] Asymptotic-preserving neural networks for kinetic equations in socio-epidemics

**Format :** Talk at Waseda University

**Author(s) :** Giulia Bertaglia (University of Ferrara)

**Abstract :** Data-driven approaches have proven to be powerful tools with a direct impact on society. However, the use of standard neural networks to investigate multiscale dynamics can lead to erroneous inferences and predictions, because the presence of small scales leads to reduced-order models that must be considered in the learning phase. In this talk, I will address these issues by presenting asymptotic-preserving neural networks, focusing on their use to study the spatial spread of epidemics.

## [04507] Many-agent systems and mean-field models for semi-supervised learning

**Format :** Talk at Waseda University

**Author(s) :** Lisa Maria Kreusser (University of Bath)Marie-Therese Wolfram (University of Warwick)

**Abstract :** In many problems in data classification, it is desirable to assign labels to points in a point cloud where a certain number of them is already correctly labeled. In this talk, we propose a microscopic ODE approach, in which information about correct labels propagates to neighbouring points. Its dynamics are based on alignment mechanisms, often used in collective and consensus models. We derive the respective continuum description, which corresponds to an anisotropic diffusion equation with a reaction term. Solutions of the continuum model inherit interesting properties of the underlying point cloud. We discuss the qualitative behaviour of solutions and exemplify the results with micro- and macroscopic simulations.

## [03820] Trends to equilibrium for nonlocal Fokker-Planck equations with discontinuous drift

**Format :** Talk at Waseda University

**Author(s) :** Mattia Zanella (University of Pavia)

**Abstract :** We study equilibration rates for nonlocal Fokker-Planck equations with time-dependent diffusion coefficient and drift, modeling the relaxation of a large swarms of agents, feeling each other in terms of their distance, towards the steady profile characterized by a uniform spreading over a finite domain. The result follows by combining entropy methods for quantifying the decay of the solution towards its quasi-stationary distribution, with the properties of the quasi-stationary profile.

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00057 (2/2) : 4D @G702 [Chair: Marie-Therese Wolfram]

## [04768] Kinetic modelling of swarming dynamics with transient leadership

**Format :** Talk at Waseda University

**Author(s) :** Giacomo Albi (University of Verona)

**Abstract :** In this talk, we will focus on swarming dynamics with topological interactions and where leaders' emergence initializes spontaneous changes of direction. In this context, we will provide a kinetic model for leader-follower dynamics with mass transfer among the two populations modeled as a transition process on a space of labels. This model allows the transition from followers to leaders and vice-versa, with scalar-valued transition rates depending on the state of the system. Furthermore, we will propose an efficient stochastic algorithm for the identification of the  $k$ -nearest neighbors at mesoscopic level, and the simulation of the swarming dynamics. Several numerical experiments are presented for different scenarios both to validate the algorithm and to study the collective dynamics.

## [02465] Kernel learning method for multiagent systems and its mean-field limit

**Format :** Talk at Waseda University

**Author(s) :** Chiara Segala (RWTH Aachen University) Michael Herty (RWTH Aachen University) Christian Fiedler (RWTH Aachen University)

**Abstract :** Kernel methods are among the most popular and successful machine learning techniques. From a mathematical point of view, these methods rest on the concept of kernels and function spaces generated by kernels. Motivated by recent developments of learning approaches in the context of interacting particle systems, we investigate kernel methods acting on data with many measurement variables. We present efficient learning algorithms both on microscopic and mean-field level.

## [03937] Bounded-confidence models of opinion dynamics on networks

**Format :** Talk at Waseda University

**Author(s) :** Heather Zinn Brooks (Harvey Mudd College)

**Abstract :** In this talk, I will introduce you to a class of models of opinion dynamics on networks called bounded-confidence models. These relatively simple models can produce delightfully complicated dynamics and provide a rich source of study for the interplay between dynamics and structure. I will discuss some novel twists on bounded-confidence models that my collaborators and I have been developing, including information cascades, bifurcations in "smoothed" bounded-confidence models, and extensions to hypergraphs.

## [03493] Mean-field models for many agent systems with co-evolving network structure

**Format :** Online Talk on Zoom

**Author(s) :** Martin Burger (DESY and University of Hamburg)

**Abstract :** In this talk we discuss the derivation of kinetic and sub mean-field equations for processes related to processes on networks, such as opinion formation on social networks. We consider in particular the case when networks are co-evolving during other processes and discuss suitable descriptions as well as issues to derive simple closure relations. Moreover, we discuss aspects of pattern formation such as consensus or the formation of echo chambers.

# [00059] Numerical solutions for differential equations: Probabilistic approaches and statistical perspectives

**Session Time & Room :**

00059 (1/2) : 1C (Aug.21, 13:20-15:00) @E503

00059 (2/2) : 1D (Aug.21, 15:30-17:10) @E503

**Type :** Proposal of Minisymposium

**Abstract :** Many applications involve predicting the dynamics of a system by solving differential equations. Due to the increased demand for predictive power of these models, numerically solving a differential equation is now often combined with parameter estimation or uncertainty quantification. This paradigm shift drives the need for probabilistic approaches that are compatible with statistical inference, or that improve the robustness of inference to possibly inaccurate mathematical models. The talks in this minisymposium will present recent work that addresses these challenges for deterministic ODEs and PDEs, by using ideas from numerical analysis, probability theory, and Bayesian statistical inference.

**Organizer(s) :** Han Cheng Lie, Takeru Matsuda, Yuto Miyatake

**Classification :** 62F15, 62G99, 65L05, 65N75

**Minisymposium Program :**


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00059 (1/2) : 1C @E503 [Chair: Han Cheng Lie]

## [00066] Probabilistic Numerical Methods

**Format :** Online Talk on Zoom

**Author(s) :** Chris Oates (Newcastle University)

**Abstract :** The scale and complexity of modern scientific computer codes typically precludes a detailed analysis of how the code is numerically implemented. For example, multi-scale and multi-physics models of the human heart call on diverse numerical sub-routines to integrate differential equations, perform interpolation and optimise over some parameters of the model. As such, the computer output is acknowledged to be inexact and some alternative form of uncertainty quantification is needed for the output to be properly interpreted. This talk will provide an introduction to probabilistic numerical methods, which aim to provide probabilistic uncertainty quantification for computer code output. These methods are composed of "modules", such that a probabilistic description of numerical error can be automatically propagated, and some of the most useful modules will be discussed.

## [04930] Prior models for enforcing boundary constraints in state-space probabilistic PDE solvers

**Format :** Online Talk on Zoom

**Author(s) :** Oksana Chkrebtii (The Ohio State University)Yue Ma (The Ohio State University)

**Abstract :** Probabilistic numerics is an active field of research that seeks to construct stochastic analogues of numerical methods, including the solution of ordinary and partial differential equations. Probabilistic solvers for partial differential equations require the specification of flexible prior models that respect physical constraints while allowing for computational efficiencies of the sequential updates. We focus on state-space based probabilistic PDE solvers and describe advances in nonparametric modeling of system states with boundary constraints.

## [04408] GParareal: Towards a time-parallel probabilistic ODE solver

**Format :** Talk at Waseda University

**Author(s) :** T J Sullivan (University of Warwick)Kamran Pentland (University of Warwick)Massimiliano Tamborrino (University of Warwick)Lynton Appel (Culham Centre for Fusion Energy)James Buchanan (Culham Centre for Fusion Energy)

**Abstract :** Numerical solution of complex ODEs can be accelerated with time-parallel integration, predicting the solution serially using a cheap solver and correcting these values in parallel using an expensive solver. We propose a time-parallel ODE solver (GParareal) that models the prediction-correction term using a Gaussian process emulator. GParareal compares favourably with the classic parareal algorithm, locates solutions to certain ODEs where parareal fails, and can also use archives of legacy solutions to further accelerate convergence.

## [00148] Theoretical Guarantees for the Statistical Finite Element Method

**Format :** Online Talk on Zoom

**Author(s) :** Yanni Papandreou (Imperial College London)Jon Cockayne (University of Southampton)Mark Girolami (University of Cambridge)Andrew B. Duncan (Imperial College London)

**Abstract :** The statistical finite element method (StatFEM) is an emerging probabilistic method that allows observations of a physical system to be synthesized with the numerical solution of a PDE intended to describe it in a coherent statistical framework, to compensate for model error. This work presents a new theoretical analysis of the statistical finite element method demonstrating that it has similar convergence properties to the finite element method on which it is based. Our results constitute a bound on the Wasserstein-2 distance between the ideal prior and posterior and the StatFEM approximation thereof, and show that this distance converges at the same mesh-dependent rate as finite element solutions converge to the true solution. Several numerical examples are presented to demonstrate our theory, including an example which test the robustness of StatFEM when extended to nonlinear quantities of interest.

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00059 (2/2) : 1D @E503 [Chair: Yuto Miyatake]

## [00714] Approximating the solutions of delay differential equations via the randomized Euler method

**Format :** Talk at Waseda University

**Author(s) :** Yue Wu (University of Strathclyde)Fabio Difonzo (University of Bari Aldo Moro)Pawel Przybyl (AGH University of Science and Technology)

**Abstract :** In this talk, we consider Caratheodory delay ODEs with time-irregular coefficients, where a randomized Euler scheme is proposed to approximate the exact solution. This is the case when there is a lack of convergence for deterministic algorithms.

## [00186] Posterior error estimates for statistical finite element methods with Sobolev priors

**Format :** Talk at Waseda University

**Author(s) :** Toni Karvonen (University of Helsinki)Fehmi Cirak (University of Cambridge)Mark Girolami (University of Cambridge)

**Abstract :** The statistical finite element, statFEM, approach synthesises measurement data with finite element models and allows for making predictions about the system response. Suppose that noisy measurement data are generated by a deterministic true system response function satisfying a second-order elliptic partial differential equation for an unknown true source term. In this setting, we provide probabilistic error analysis for a prototypical statFEM setup based on a Gaussian process prior whose covariance kernel induces a Sobolev space.

## [04863] The Bayesian approach to inverse Robin problems

**Format :** Talk at Waseda University

**Author(s) :** Ieva Kazlauskaitė (University of Cambridge)

**Abstract :** In this talk, I will present the Bayesian approach to inverse Robin problems. The problem of interest is a certain elliptic boundary value problem of determining a Robin coefficient on a hidden part of the boundary from Cauchy data on the observable part. Such an inverse problem arises naturally in the initialisation of large-scale ice sheet models that are crucial in climate and sea-level predictions. We motivate the Bayesian approach for a prototypical Robin inverse problem by showing that the posterior mean converges in probability to the data-generating ground truth as the number of observations increases. Related to the stability theory for inverse Robin problems, we establish a logarithmic convergence rate for regular Robin coefficients, whereas for analytic coefficients we can attain an algebraic rate. Further, our numerical results demonstrate the effectiveness of the approach in recovering the Robin coefficient for an ice sheet model.

## [02954] Statistical finite elements for misspecified models

**Format :** Talk at Waseda University

**Author(s) :** Connor Duffin (University of Cambridge)Edward Cripps (University of Western Australia)Thomas Stemler (University of Western Australia)Mark Girolami (University of Cambridge)

**Abstract :** I will present a statistical finite element method for nonlinear, time-dependent problems. This is a statistical augmentation of the finite element method which admits model misspecification inside of the governing equations, via Gaussian processes. The method is Bayesian, sequentially updates model mismatch upon receipt of observed data, and ensures scalability through low-rank approximations to the posterior. In this talk I will present statFEM and discuss various case studies with experimental and synthetic data.

# [00060] Mathematical approaches to collective phenomena

**Session Time & Room :** 3C (Aug.23, 13:20-15:00) @E803

**Type :** Proposal of Industrial Minisymposium

**Abstract :** The contributions of the mathematics to understanding of collective phenomena such as the fluid dynamics are certainly conspicuous. In particular, developments of the numerical method to solve PDE, PDE analysis of the hydrodynamic equation or Boltzmann equation by applied mathematicians are quite significant in the industry. This minisymposium invites four eminent researchers, who study various types of collective phenomena such as the gas dynamics, biological swarming, electrically charged fluids and so on. Their presentations will indicate new insights and inspirations in the future applied mathematics.

**Organizer(s) :** Ryosuke Yano

**Classification :** 65Z05, 65N06, 70-10, 92-10

**Minisymposium Program :**

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00060 (1/1) : 3C @E803 [Chair: Ryosuke Yano]

## [04763] Multi-fidelity method for a class of kinetic equations with uncertainties

**Format :** Talk at Waseda University

**Author(s) :** Liu Liu (The Chinese University of Hong Kong )Lorenzo Pareschi (University of Ferrara)xueyu zhu (University of Iowa)

**Abstract :** In this talk, we will discuss some recent development on the topic of multi-fidelity methods for solving a class of kinetic equations with uncertainties and multiple scales. The Boltzmann equation, linear transport equation and epidemic transport system will be particularly studied, together with formal error estimates. We will also briefly discuss application of deep learning approaches to study kinetic problems.

## [04788] Brownian HydroDynamics for Confined Electrolyte Solutions

**Format :** Talk at Waseda University

**Author(s) :** Aleksandar Donev (Courant Institute, New York University)

**Abstract :** Electrolyte solutions appear in many engineering systems and processes, such as desalination, microfluidic pumps, and batteries. For confined electrolytes, (quasistatic) long-ranged electrostatic interactions among the particles play a crucial role in the static structure. Similarly, hydrodynamic interactions (HIs) mediated by the solvent are also long-ranged and affect the dynamics in crucial ways. Confinement in slit channel geometries is of particular importance, especially for electrohydrodynamics and electrochemistry near electrodes in devices and batteries. In particular, very thin electric (Debye) double layers with complex structure form near dielectric or metallic boundaries and many important electro-hydrodynamic phenomena occur in this layer. I will discuss the limitations of the classical Poisson-Nernst-Planck-Stokes equations for non-dilute electrolytes, in which the Debye scale is molecular, and present an alternative Brownian HydroDynamics (BD-HI) approach that uses fluctuating hydrodynamics for the solvent but represents the ions as explicit Brownian particles. By using BD-HI we are able to reach much longer (diffusive) time scales than molecular dynamics because of the implicit overdamped solvent, at the expense of loosing some microscopic details.

## [04809] Delay Models of Collective Behavior with Biological and Industrial Applications

**Format :** Talk at Waseda University

**Author(s) :** Jan Haskovec (King Abdullah University of Science and Technology)

**Abstract :** The talk will give an overview of recent results for models of collective behavior governed by delay differential equations. It will focus on models of interacting agents with applications in biology (flocking, swarming), social sciences (opinion formation) and engineering (swarm robotics), where latency (delay) plays a significant role. We will explain that there are two main sources of delay - inter-agent communications and information processing - and show that they have qualitatively different impacts on the group dynamics. We will give an overview of analytical methods for studying the asymptotic behavior of the models and their mean-field limits. Finally, motivated by situations where finite speed of information propagation is significant, we will introduce an interesting class of problems where the delay depends nontrivially and nonlinearly on the state of the system, and discuss the available analytical results and open problems here.

## [04973] Model Cascades for Dilute Gases Based on Moment Equations

**Format :** Talk at Waseda University

**Author(s) :** Manuel Torrilhon (RWTH Aachen)

**Abstract :** Dilute gas flows show thermal non-equilibrium due to lack of particle collisions. This requires modeling using the statistical description of kinetic gas theory. Moment equations extend the classical fluid dynamic equations for processes with moderate Knudsen numbers. We will present non-equilibrium models based on moment approximations, which provide a hierarchy of models in a cascading nature. This can be used to estimate model errors and perform model-adaptive simulations.

## [00061] Reaction-Diffusion models in Ecology and Evolution

**Session Time & Room :**

00061 (1/2) : 3C (Aug.23, 13:20-15:00) @G602

00061 (2/2) : 3D (Aug.23, 15:30-17:10) @G602

**Type :** Proposal of Minisymposium

**Abstract :** Reaction-diffusion equations have been a powerful tool in studying population dynamics since the seminal works of Fisher, Kolmogorov-Petrovsky-Piskunov, Turing, and many others. In recent years many important questions from ecology, such as habitat fragmentation and shifting environment change, and life sciences, such as tumor growth, required new mathematical models and gave rise to challenging problems in analysis. This mini-symposium aims to showcase some recent development in the theory of reaction-diffusion equations and its applications to some emerging ecological and evolutionary questions.

**Organizer(s) :** King-Yeung Lam, Yuan Lou, Dongyuan Xiao, Maolin Zhou

**Classification :** 35K57, 35C07

**Minisymposium Program :**

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00061 (1/2) : 3C @G602 [Chair: King-Yeung Lam]

## [00123] Propagation direction of the traveling wave in the Lotka-Volterra competition-diffusion system

**Format :** Talk at Waseda University

**Author(s) :** Chiun-Chuan Chen (National Taiwan University)

**Abstract :** We consider the two species Lotka-Volterra competition-diffusion system and assume that the species are in strong competition. It is well-known that up to a translation, there exists a unique monotone traveling wave solution. The sign of the wave speed provides significant information about which species can wipe out the other. However, it is a difficult problem to determine the sign of the speed. In this talk, we will present some estimates for the relation between the wave speed and the growth rates of the species. With these estimates, we are able to determine the speed sign under some suitable conditions.

## [00124] Principal eigenvalue problem with large advection in 2 dimensional case

**Format :** Talk at Waseda University

**Author(s) :** Maolin Zhou (Nankai University)

**Abstract :** In this talk, we will discuss the recent progress on the limit of the principal eigenvalue of some second order operators with large advection: 1. degenerate case; 2. parabolic case (1-d); 3. elliptic case (2-d).

## [00099] Some game theoretical models in population dynamics

**Format :** Talk at Waseda University

**Author(s) :** Idriss Mazari-Fouquer (CEREMADE, Paris Dauphine Université, PSL)

**Abstract :** We review several recent contributions aimed at providing a better understanding of optimal fishing strategies in spatial ecology: how should one fish in order to maximise the fishing output? If several players are fishing, can they reach an equilibrium situation? Formulated in terms of optimal control problems and Nash equilibria properties, these problems are amenable to mathematical analysis, and we present a variety of related results. Joint work with D. Ruiz-Balet.

## [00125] Free boundary problem for the curve shortening flow with driving force in undulating cylindrical domains

**Format :** Talk at Waseda University

**Author(s) :** Ryunosuke Mori (Meiji University)

**Abstract :** We study a free boundary problem for the curve shortening flow with driving force in a two-dimensional cylindrical domain with periodically undulating boundary. We consider the large time behavior of the graph-like solution. The classical solution generally does not exist in global time, since the solution may touch the boundary of the domain in finite time. To overcome this difficulty, we prove that the set of singularities of the solution is discrete under some assumptions.

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00061 (2/2) : 3D @G602 [Chair: Maolin Zhou]

## [00120] Front Propagation in the Shadow Wave-Pinning Model

**Format :** Talk at Waseda University

**Author(s) :** Daniel Gomez (University of Pennsylvania)King-Yeung Lam (The Ohio State University)Yoichiro Mori (University of Pennsylvania)

**Abstract :** In this paper we consider a non-local bistable reaction-diffusion equation arising from cell polarization. A typical solution of this model exhibits an interface with velocity regulated by the total mass. The feedback between mass-conservation and bistability causes the interface to approach a fixed limit. In the limit of a small diffusivity  $\varepsilon^2 \ll 1$ , we prove that for any  $0 < \gamma < 1/2$  the interface can be estimated within  $O(\varepsilon^\gamma)$  of the location as predicted using formal asymptotics.

## [00109] Propagation speeds in a shifting environment

**Format :** Talk at Waseda University

**Author(s) :** Thomas Giletti (University of Lorraine)

**Abstract :** I will discuss the asymptotic behavior of solutions of reaction-diffusion equations with shifting heterogeneity. Such a situation arises in the modeling of population dynamics under an environmental change, due to global warming or the invasion by competing species. Two situations will be considered, depending on whether the reaction or the diffusion is heterogeneous. We will see that the heterogeneity may modify the nature of the propagation by inducing some unexpected threshold or acceleration phenomena.

## [00067] Lotka-Volterra competition-diffusion system: the critical competition case

**Format :** Talk at Waseda University

**Author(s) :** Dongyuan XIAO (Meiji University)Matthieu Alfaro (Universite de Rouen Normandie)

**Abstract :** We consider the competition system in the so-called critical competition case. The associated ODE system then admits infinitely many equilibria. We first show the non-existence of ultimately monotone traveling waves. Next, we study the large-time behavior of the solution of the Cauchy problem with a compactly supported initial datum and provide a sharp description of the profile of the solution.

## [00080] Coexistence of strains in some reaction-diffusion systems for infectious disease

**Format :** Talk at Waseda University

**Author(s) :** Lou Yuan (Shanghai Jiao Tong University)Rachidi Salako (University of Nevada at Las vegas)

**Abstract :** We study the global dynamics of some reaction-diffusion systems for multiple strains and investigate how the coexistence of strains is impacted by the movement of populations and spatial heterogeneity of the environment. For the case of two strains, general conditions for the existence, uniqueness and stability of coexistence steady states are found. Surprisingly, when there is no coexistence of strains, it is possible for the weak strain to be dominant for intermediate diffusion rates, in strong contrast to small and large diffusion cases where the weak strain goes extinct.

# [00062] Analysis and computation of vortical flows

## Session Time & Room :

00062 (1/3) : 1C (Aug.21, 13:20-15:00) @D102

00062 (2/3) : 1D (Aug.21, 15:30-17:10) @D102

00062 (3/3) : 1E (Aug.21, 17:40-19:20) @D102

## Type : Proposal of Minisymposium

**Abstract :** Vortex dynamics is a classical but ever active topic in the study of fluid flows. Despite huge efforts to understand vortex phenomena, many aspects are still not properly understood. In this minisymposium, Elling and Jeong are presenting mathematical and rigorous results of self-similar vortices. Xu will describe computations of elliptical vortices. Kim and Krishnamurthy will discuss point vortex dynamics and generalized geostrophic models. Nitsche and Sohn speak on computational issues for interfacial flows and application to swimming. Krasny will present computations of plasma vortices in the Vlasov-Poisson equation.

**Organizer(s) :** Sun-Chul Kim, Robert Krasny, Sung-Ik Sohn

**Classification :** 76B47, 76E17, 76B03, 76U60, 35Q83

## Minisymposium Program :

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00062 (1/3) : 1C @D102 [Chair: Sun-Chul Kim]

## [00106] Logarithmic vortex spirals

### Format : Talk at Waseda University

**Author(s) :** In-Jee Jeong (Seoul National University)

**Abstract :** We investigate the dynamics of logarithmic vortex for the two-dimensional incompressible Euler equations. More precisely, we consider vorticity which is invariant under the transformation  $(r, \theta) \mapsto (\lambda r, \theta + c \ln(\lambda))$  for any  $\lambda > 0$  and some  $c > 0$ . Within this class of vorticities, one can consider various types, including patches and sheets. We derive the equations of motion for logarithmic vortex and consider the limit problem where patches become sheets.

## [00069] Dynamics of elliptical vortices

### Format : Online Talk on Zoom

**Author(s) :** Ling Xu (North Carolina Agricultural and Mechanical State University)Robert Krasny (University of Michigan, Ann Arbor)

**Abstract :** We examine the dynamics of elliptical vortices in 2D ideal fluid using an adaptively refined and remeshed vortex method. Four cases are considered: the compact MMZ and POLY vortices, and noncompact Gaussian and smooth Kirchhoff vortices (SK). The vortices have the same maximum vorticity and 2:1 initial aspect ratio, but unlike the top-hat Kirchhoff vortex, they have continuous profiles with different regularity. In all cases the co-rotating phase portrait has two hyperbolic points. At early time two filaments emerge and form a halo around the core as vorticity is advected along the unstable manifold of each hyperbolic point. The Gaussian vortex rapidly axisymmetrizes, but later on the core begins to oscillate and two small lobes emerge adjacent to the core; this is attributed to a resonance. For the MMZ, POLY, and SK vortices, the core maintains its ellipticity for longer time and the filaments entrain fluid into two large lobes forming a non-axisymmetric tripole state; afterwards the lobes repeatedly detrain fluid into the halo; this is attributed to a heteroclinic tangle. While prior work suggested that elliptical vortices evolve to either an axisymmetric state or a non-axisymmetric tripole state, our results suggest that such vortices may oscillate between these states.

## [00121] The N-vortex problem in doubly-periodic domains with background vorticity

### Format : Talk at Waseda University

**Author(s) :** Vikas Krishnamurthy (IIT Hyderabad)Takashi Sakajo (Kyoto University)

**Abstract :** We study the N-vortex problem in a doubly periodic rectangular domain in the presence of a constant background vorticity field. Using a conformal mapping approach, we derive an explicit formula for the hydrodynamic Green's function. We show that the point vortices form a Hamiltonian system and that the two-vortex problem is integrable. Several fixed lattice configurations are obtained for general N, some of which consist of vortices with inhomogeneous strengths and lattice defects.

## [00127] Swimming of a Fish-like Body by using a Vortex Shedding Model

**Format :** Talk at Waseda University

**Author(s) :** SUNG-IK SOHN (Gangneung-Wonju National University)

**Abstract :** We consider the undulatory motion of a body translating through a quiescent fluid, which is motivated by the anguilliform swimming of aquatic animals, e.g., eels. We use an inviscid vortex shedding model to investigate the swimming dynamics. The model demonstrates the self-propulsion of the swimming body and yields pairs of anti-rotating vortices shed from the body. We examine the wake pattern and swimming efficiency which depends on the recoil motions of a body.

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00062 (2/3) : 1D @D102 [Chair: Sung-Ik Sohn]

## [00075] Motion of three geostrophic vortices

**Format :** Talk at Waseda University

**Author(s) :** Sun-Chul Kim (Chung-Ang University, Seoul, Korea (Republic of))Habin Yim (Chung-Ang University, Seoul, Korea (Republic of))Sung-Ik Sohn (Gangneung-Wonju National University)

**Abstract :** We investigate the dynamics of geostrophic Bessel vortices focusing on the three-vortex case, where the possibility of self-similar motion and general dynamics for arbitrary strengths is studied. It is found that self-similar motions are limited to rigid rotations and self-similar triple collapse is impossible. For a general description, trilinear coordinates are adopted. The physical regions in the phase plane cannot be directly identified, but the boundary approaches the vertices of the triangle in trilinear coordinates in geostrophic vortices.

## [00126] Self-similar vortical flows

**Format :** Talk at Waseda University

**Author(s) :** Volker Wilhelm Elling (Academia Sinica, Taipei)

**Abstract :** Vortex spirals and vortex cusps are important features of self-similar vortical flows near stagnation points. Vortex sheets produced at triple points of Mach reflection have distinguished signs that determine whether interaction with walls or symmetry axes can be attached cusps or detached jets. Progress on analysis, modelling and numerics for such phenomena is discussed, along with applications to shock reflection or non-uniqueness of vortical flows.

## [00150] Near-singular integrals in 3D interfacial Stokes and potential flows

**Format :** Talk at Waseda University

**Author(s) :** Monika Nitsche (University of New Mexico)

**Abstract :** Boundary integral formulations yield efficient numerical methods to solve elliptic boundary value problems. They are the method of choice for interfacial fluid flow in either the inviscid vortex sheet limit, or the viscous Stokes limit. The fluid velocity at a target point is given by an integral over all interfaces. However, for target points near, but not on the interface, the integrals are near-singular and standard quadratures lose accuracy. While several accurate methods for near-singular integrals exist in planar geometries, they do not generally apply to the non-analytic case that arises in axisymmetric or 3D geometries. We present a method based on Taylor series expansions of the integrand about basepoints on the interface that accurately resolve a large class of integrals, and apply it to solve the near-interface problem in planar vortex sheet flow, axisymmetric Stokes flow, and Stokes flow in 3D. The application to multi-nested Stokes flow uses a novel representation of the fluid velocity.

## [00147] The FARSIGHT Vlasov-Poisson code

**Format :** Talk at Waseda University

**Author(s) :** Robert Krasny (University of Michigan)Ryan Sandberg (Lawrence Berkeley National Laboratory)Alexander Thomas (University of Michigan)

**Abstract :** We present electrostatic plasma simulations using a new semi-Lagrangian particle method for the Vlasov-Poisson equations called FARSIGHT. The electron density is represented on adaptively refined and remeshed panels in phase space, and the macroparticles are advected using a regularized electric field kernel and a GPU-accelerated barycentric Lagrange treecode. Results are presented for Landau damping, two-stream instability, and ion beam propagation. Work supported by AFOSR grant FA9550-19-1-0072.

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00062 (3/3) : 1E @D102

# [00063] Recent Advances on Nonlocal Interaction Models

**Session Time & Room :**

00063 (1/4) : 1E (Aug.21, 17:40-19:20) @F311

00063 (2/4) : 2C (Aug.22, 13:20-15:00) @F311

00063 (3/4) : 2D (Aug.22, 15:30-17:10) @F311

00063 (4/4) : 2E (Aug.22, 17:40-19:20) @F311

**Type :** Proposal of Minisymposium

**Abstract :** From biological swarming and n-body dynamics to self-assembly of nanoparticles, crystallization and granular media, many physical and biological systems are described by mathematical models involving nonlocal interactions. Mostly due to their purely nonlocal character, these models present mathematical challenges that require a combination of different techniques of applied mathematics. With this scientific session we aim to bring together young researchers and leading scholars who study nonlocal interaction models and their applications. In particular, we hope that by inviting applied and pure analysts we will create a platform that will lead to a more complete and reliable understanding of these models.

**Organizer(s) :** Razvan Fetecau, Ihsan Topaloglu

**Classification :** 45K05, 35A15, 70F99, 82B21, Nonlocal Partial Differential Equations

**Minisymposium Program :**


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00063 (1/4) : 1E @F311

## [04295] Patterns in block copolymers

**Format :** Talk at Waseda University

**Author(s) :** Stan Alama (McMaster University)Lia Bronsard (McMaster University)Xin Yang Lu (Lakehead University)Chong Wang (Washington and Lee University)

**Abstract :** We study a nonlocal isoperimetric problem for several interacting phase domains which consists of a local interface energy and of a longer-range Coulomb interaction energy. We consider global minimizers on the two-dimensional torus, in a limit in which some of the species have vanishingly small mass. Depending on the relative strengths of the coefficients we may see different structures for the global minimizers. This represents work with S. Alama, X. Lu, and C. Wang.

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00063 (2/4) : 2C @F311 [Chair: Ihsan Topaloglu]

## [00152] Patterns in tri-block copolymers: droplets, double-bubbles and core-shells.

**Format :** Talk at Waseda University

**Author(s) :** Stan Alama (McMaster Univ)Lia Bronsard (McMaster University)Xin Yang Lu (Lakehead Univ)Chong Wang (Washington and Lee Univ)

**Abstract :** We study the Nakazawa-Ohta ternary inhibitory system, which describes domain morphologies in a triblock copolymer as a nonlocal isoperimetric problem for three interacting phase domains. The free energy consists of two parts: the local interface energy measures the total perimeter of the phase boundaries, while a longer-range Coulomb interaction energy reflects the connectivity of the polymer chains and promotes splitting into micro-domains. We consider global minimizers on the two-dimensional torus, in a limit in which two of the species have vanishingly small mass but the interaction strength is correspondingly large. In this limit there is splitting of the masses, and each vanishing component rescales to a minimizer of an isoperimetric problem for clusters in 2D. Depending on the relative strengths of the coefficients of the interaction terms we may see different structures for the global minimizers, ranging from a lattice of isolated simple droplets of each minority species to double-bubbles or core-shells. This represents work with S. Alama, X. Lu, and C. Wang.

## [00113] Ground states for aggregation-diffusion models on Cartan-Hadamard manifolds

**Format :** Talk at Waseda University

**Author(s) :** Hansol Park (Simon Fraser University)

**Abstract :** We investigate the existence of ground states of a free energy functional defined on Cartan-Hadamard manifolds. There are two competing effects in the free energy: repulsion modelled by linear diffusion and attraction modelled by a nonlocal interaction term. Nonexistence of energy minimizers can occur if either the diffusion is too strong (spreading) or attraction is dominant (blow-up). Variational approaches have been used to provide sufficient conditions of the attractive interaction to prevent the two scenarios from happening, and thus establishing the existence of global minimizers of the free energy.

## [00101] Well-posedness and asymptotic behaviour of an interaction model on Riemannian manifolds

**Format :** Talk at Waseda University

**Author(s) :** Razvan C Fetecau (Simon Fraser University)

**Abstract :** We consider a model for collective behaviour with intrinsic interactions on Riemannian manifolds. We establish the well-posedness of measure solutions and study the long-time behaviour of solutions. For the latter, the primary goal is to establish sufficient conditions for a consensus state to form asymptotically. The analytical results are illustrated with numerical experiments that exhibit various asymptotic patterns.

## [00131] Mean field games with aggregating interaction potentials of nonlocal type

**Format :** Talk at Waseda University

**Author(s) :** Annalisa Cesaroni (University of Padova)

**Abstract :** We discuss existence/non existence of solutions to ergodic mean field game systems in the whole space with interactions of aggregative Riesz type, in dependance on the strength of the interaction term. Moreover, we present qualitative properties of the solutions and concentration phenomena, as the diffusion term vanishes. Finally we discuss some open problems related to stability of equilibria.

00063 (3/4) : 2D @F311 [Chair: Hansol Park]

## [00105] Deterministic particle approximation for a nonlocal interaction equation with repulsive singular potential

**Format :** Talk at Waseda University

**Author(s) :** Marco Di Francesco (University of L'Aquila)Markus Schmidtchen (TU Dresden)

**Abstract :** We consider a variant of a deterministic particle approximation for a nonlocal interaction equation with repulsive Morse potential in 1d, which is not covered by previous similar results in the literature. We prove convergence in a weak sense towards solutions to the corresponding continuum PDE. We prove our scheme is able to capture  $L^p$  contractivity and a smoothing effect which allows to extend the result to initial data in the set of probability measures.

## [00155] Nonlocal deterministic and stochastic models for collective movement in biology

**Format :** Talk at Waseda University

**Author(s) :** Raluca EFTIMIE (University of Franche-Comté)

**Abstract :** The collective movement of animals occurs as a result of communication between the members of the community. However, inter-individual communication can be affected by the stochasticity of the environment, leading to changes in the perception of neighbours and subsequent changes in individual behaviour, which then influence the overall behaviour of the animal aggregations. To investigate the effect of noise on the overall behaviour of animal aggregations, we consider a class of nonlocal hyperbolic models for the collective movement of animals. We show numerically that for some sets of model parameters associated with individual communication, strong noise does not influence the spatio-temporal pattern (i.e., travelling aggregations) observed when all neighbours are perceived with the same intensity (i.e., the environment is homogeneous). However, when neighbours ahead/behind are perceived differently by a reference individual, noise can lead to the destruction of the spatio-temporal pattern.

## [00117] Zero-Inertia Limit: from Particle Swarm Optimization to Consensus-Based Optimization

**Format :** Talk at Waseda University

**Author(s) :** Hui Huang (University of Graz)

**Abstract :** Large systems of interacting particles are widely used to investigate self-organization and collective behavior. They have also been used in metaheuristic methods, which can provide empirically robust solutions to tackle hard optimization problems with fast algorithms. In this talk, we will focus on two examples of metaheuristics, i.e. Particle Swarm Optimization (*PSO*) and Consensus-Based Optimization (*CBO*). In particular, we shall provide a rigorous derivation of *CBO* from *PSO* through the limit of zero inertia. This is also related to the problems of overdamped limit and large-friction limit.

## [00093] Many-spike limits of reaction-diffusion systems of PDEs

**Format :** Talk at Waseda University

**Author(s) :** Theodore Kolokolnikov (Dalhousie University)

**Abstract :** Many reaction-diffusion have solutions consisting of spots or spikes. We consider the problem of describing the density distribution of these spikes when the number of spikes is large. This naturally leads to integral equation for spike density.

00063 (4/4) : 2E @F311 [Chair: Razvan C Fetecau]

## [00157] Pattern formation in particle systems: spherical shells to regular simplices

**Format :** Talk at Waseda University

**Author(s) :** Robert John McCann (University of Toronto, Department of Mathematics)

**Abstract :** Flocking and swarming models address mathematical biological pattern formation. When organisms interact through a difference of power laws attractive over large distances yet repulsive at short distances, we detail a phase transition which separates a region where the minimum energy configuration is uniquely attained by a uniform distribution of organisms over a spherical shell, from a region in which it is uniquely attained by equidistributing the organisms over the vertices of a regular top-dimensional simplex.

## [05071] Some remarks on minimization of nonlocal attracting repulsing energies

**Format :** Online Talk on Zoom

**Author(s) :** Aldo Pratelli (University of Pisa)Ihsan Topaloglu (Virginia Commonwealth University)Davide Carazzato (SNS, Pisa)Nicola Fusco (University of Naples)

**Abstract :** We will discuss some results on the minimization of nonlocal energies of attraction-repulsion type. In particular, we will be interested in existence and regularity of minimizing sets, and of generalised solutions, i.e., functions or measures. Some of the presented results are well-known, some others are recent or very recent developments. Some of the results have been obtained in various collaborations with D. Carazzato, N. Fusco, I. Topaloglu.

## [00145] On a Becker-Döring model for prions and an associated nonlocal problem.

**Format :** Online Talk on Zoom

**Author(s) :** Klemens Fellner (University of Graz)

**Abstract :** Prions are able to self-propagate biological information through the transfer of structural information from a misfolded/infectious protein in a prion state to a protein in a non-prion state. Prions cause diseases like Creuzfeldt-Jakob. Prion-like mechanisms are associated to Alzheimer, Parkinson and Huntington diseases. We present a fundamental bimolecular, nonlinear Becker-Döring type model, which aims to explain experiments in the lab of Human Rezaei showing sustained oscillatory behaviour over multiple hours. We exemplify a mechanism of oscillatory behaviour and show numerical simulations. An interesting non-local problem describes an associated self-similar structure.

## [04453] Shape Optimization for nonlocal anisotropic energies

**Author(s)** : Lucia Scardia (Heriot-Watt University)

**Abstract** : We address the problem of shape optimisation for sets with fixed mass, in the case of attractive-repulsive nonlocal energies. More precisely, we focus on energies whose repulsive part is an anisotropic Newtonian potential, and whose attractive part is radially symmetric, and quadratic.

For the fully radially symmetric case, it is known that the existence of minimisers depends on the value of the mass: there is a critical value such that minimisers are balls above it, and do not exist below it. We show that a similar dichotomy occurs also in the anisotropic case. The anisotropy, however, introduces an additional critical value that makes the analysis subtle.

This is work in collaboration with Riccardo Cristoferi and Maria Giovanna Mora.

## [00065] Recent Advances on Stochastic Hamiltonian Dynamical Systems

**Session Time & Room :**

00065 (1/3) : 2C (Aug.22, 13:20-15:00) @E819

00065 (2/3) : 2D (Aug.22, 15:30-17:10) @E819

00065 (3/3) : 2E (Aug.22, 17:40-19:20) @E819

**Type** : Proposal of Minisymposium

**Abstract** : The generalization of classical geometric mechanics ( including the study of symmetries, Hamiltonian and Lagrangian mechanics, and the Hamilton-Jacobi theory, etc.) to the context of stochastic dynamics has drawn more and more attention in recent decades. One of the important motivations behind some pieces of work related to this field is establishing a framework adapted to the handling of mechanical systems subjected to random perturbations or whose parameters are not precisely determined and are hence modeled as realizations of a random variable. This minisymposium will bring together speakers with diverse but related background, discussing recent developments on general topics of stochastic dynamical systems with Hamiltonian or other geometric structure.

**Organizer(s)** : Pingyuan Wei, Qiao Huang

**Classification** : 70L10, 37H05, 37J65, 70H05, 70H09

**Minisymposium Program :**

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00065 (1/3) : 2C @E819

## [04102] The Hamilton-Jacobi Theory for Stochastic Hamiltonian Systems on Jacobi Manifold

**Format** : Talk at Waseda University

**Author(s)** : Pingyuan Wei (Beijing International Center for Mathematical Research, Peking University, Beijing 100871, China)Qiao Huang (Nanyang Technological University)

**Abstract** : In this talk, we generalize the systems of Hamiltonian diffusions, which were introduced and studied by Bismut, to accommodate arbitrary Jacobi manifolds as phase spaces and general continuous semimartingales as forcing noises. As is well-known, Jacobi structures are the natural generalization of Poisson structure and in particular of symplectic, cosymplectic and Lie-Poisson structures. However, very interesting manifolds like contact and locally conformal symplectic manifolds are also Jacobi but not Poisson. We are interested in the systems such that the phase flows preserve characteristic structures, and develop a Hamilton-Jacobi theory which is regarded as an alternative method for formulating the dynamics. A particular example is the case of thermodynamic dynamics in which we apply our methods on a manifold with its canonical contact form.

## [02876] Homogenization of Dissipative Hamiltonian Systems under L'evy Fluctuations

**Format** : Talk at Waseda University

**Author(s)** : Zibo Wang (Huazhong University of Science and Technology)

**Abstract** : We study the small mass limit for a class of Hamiltonian systems with multiplicative non-Gaussian L'evy noise. The limiting equation has a discontinuous noise-induced drift term. First, we show that the momentum in the stochastic Hamiltonian system converges to zero when the kinetic energy has polynomial growth. Then we prove that

the stochastic Hamiltonian system with classical kinetic energy converges to the limiting equation in probability with respect to Skorohod topology.

## [02877] The stochastic flocking model with far-field degenerate communication

**Format :** Talk at Waseda University

**Author(s) :** Li Lv (Huazhong University of Science and Technology)

**Abstract :** We reconsider the stochastic kinetic Cucker-Smale model with multiplicative Brownian noise, in which we remove the positive lower bound assumption on the communication. First we prove the emergence of conditional flocking in strong sense. Then, we show that unconditional strong flocking occurs when communication weight decays slowly at the far field. These results imply uniform stability and mean-field limit. In particular, strong stability and mean-field limit in the expectation sense are established in one-dimensional case.

## [04106] The Most Likely Transition Path for a Class of Distribution-Dependent Stochastic Systems

**Format :** Talk at Waseda University

**Author(s) :** Wei Wei (Shanghai Jiao Tong University) Jianyu Hu (Nanyang Technological University)

**Abstract :** Distribution-dependent stochastic dynamical systems arise widely in engineering and science. We consider a class of such systems which model the limit behaviors of interacting particles moving in a vector field with random fluctuations. We aim to examine the most likely transition path between equilibrium stable states of the vector field. In the small noise regime, we find that the action functional (or rate function) does not involve with the solution of the skeleton equation, which describes unperturbed deterministic flow of the vector field shifted by the interaction at zero distance. As a result, we are led to study the most likely transition path for a stochastic differential equation without distribution-dependency. This enables the computation of the most likely transition path for these distribution-dependent stochastic dynamical systems by the adaptive minimum action method and we illustrate our approach in two examples.

00065 (2/3) : 2D @E819

## [00862] A parameterization method for quasi-periodic systems with noise

**Format :** Talk at Waseda University

**Author(s) :** Lei Zhang (Dalian University of Technology) Pingyuan Wei (Beijing International Center for Mathematical Research, Peking University)

**Abstract :** This work is devoted to studying the existence of invariant tori for a class of quasi-periodically forced systems with stochastic noise, and implementing an efficient method to compute the tori as well as Lyapunov exponents. These systems are skew-product systems driven by small perturbations. Two very common cases of noise included in our treatment are continuous stationary stochastic process and white noise. The existence of invariant tori is established by developing a parameterization method in random setting and applying an elementary fixed point theorem in Banach spaces. Based on this, we describe a numerical algorithm for the computation of them. Moreover, by considering the reducibility for random manifold, we also propose a numerical algorithm for the computation of the corresponding Lyapunov exponents.

## [04265] Parametric Resonance for Enhancing the Rate of Metastable Transition

**Format :** Talk at Waseda University

**Author(s) :** Ying Chao (Xi'an Jiaotong University) Molei Tao (Georgia Institute of Technology)

**Abstract :** In this talk, we will introduce a way to quantify how periodic perturbation can change the rate of metastable transition in stochastic mechanical systems with weak noises. A closed-form explicit expression for approximating the rate change is provided, and the corresponding transition mechanism can also be approximated. Unlike the majority of existing relevant works, these results apply to kinetic Langevin equations with high-dimensional potentials and nonlinear perturbations. They are obtained based on a higher-order Hamiltonian formalism and perturbation analysis for the Freidlin-Wentzell action functional. This tool allowed us to show that parametric excitation at a resonant frequency can significantly enhance the rate of metastable transitions. Numerical experiments for both low-dimensional toy models and a molecular cluster are also provided. For the latter, we show that vibrating a material appropriately can help heal its defect, and our theory provides the appropriate vibration.

## [04127] An end-to-end deep learning approach for extracting stochastic dynamical systems with $\alpha$ -stable Lévy noise

**Format :** Talk at Waseda University

**Author(s) :** Cheng Fang (Huazhong University of Science and Technology)Yubin Lu (Illinois Institute of Technology)Ting Gao (Huazhong University of Science and Technology)Jinqiao Duan (Great Bay University)

**Abstract :** Recently, extracting data-driven governing laws of dynamical systems through deep learning frameworks has gained a lot of attention in various fields. Moreover, a growing amount of research work tends to transfer deterministic dynamical systems to stochastic dynamical systems, especially those driven by non-Gaussian multiplicative noise. However, lots of log-likelihood based algorithms that work well for Gaussian cases cannot be directly extended to non-Gaussian scenarios which could have high error and low convergence issues. In this work, we overcome some of these challenges and identify stochastic dynamical systems driven by  $\alpha$ -stable Lévy noise from only random pairwise data. Our innovations include: (1) designing a deep learning approach to learn both drift and diffusion coefficients for Lévy induced noise with  $\alpha$  across all values, (2) learning complex multiplicative noise without restrictions on small noise intensity, (3) proposing an end-to-end complete framework for stochastic systems identification under a general input data assumption, that is,  $\alpha$ -stable random variable. Finally, numerical experiments and comparisons with the non-local Kramers-Moyal formulas with moment generating function confirm the effectiveness of our method.

00065 (3/3) : 2E @E819

## [04130] Schrodinger Meets Onsager

**Format :** Online Talk on Zoom

**Author(s) :** Qiao Huang (Nanyang Technological University)

**Abstract :** In this talk, we will use the framework of stochastic geometric mechanics to describe relations between Schrodinger's variational problem and Onsager's approach to nonequilibrium statistical mechanics. Especially, we will rebuild Onsager's reciprocal relations by introducing Riemannian structures on thermodynamic spaces, and propose a definition of entropy for nonequilibrium systems. This is joint work with Jean-Claude Zambrini.

## [00806] Recent progress in spatial isosceles three body problem

**Format :** Online Talk on Zoom

**Author(s) :** Lei Liu (Peking University)

**Abstract :** Recently, we discovered some new and strong connections between the spatial isosceles three body problem and Symplectic Dynamics. From this perspective, more information can be obtained. Therefore, under the light of Symplectic Dynamics, we obtain plenty of new results. In this talk, we will introduce the isosceles three body problem in symplectic and dynamical point of view, including the dimensional reduction, dynamical analysis, index estimates, open book decomposition and convexity. Finally, I will prove the existence of infinite many oscillate periodic motions in certain parametrical setting.

# [00068] Models for collective behavior and emergent phenomena

**Session Time & Room :**

00068 (1/3) : 2D (Aug.22, 15:30-17:10) @G501

00068 (2/3) : 2E (Aug.22, 17:40-19:20) @G501

00068 (3/3) : 3C (Aug.23, 13:20-15:00) @G501

**Type :** Proposal of Minisymposium

**Abstract :** Emergent structures are patterns arising via collective actions of many individual entities. In the context of life sciences, they range from the subatomic level to the entire anthropo- and biosphere. The main objective of this minisymposium is to bring together experts working in diverse areas of modeling of collective behavior and emergent phenomena, employing ordinary, stochastic, partial and functional differential equations. Applications include self-organizing systems of interacting agents, flocking and swarming, pedestrian dynamics, and network dynamics. The minisymposium will cover mathematical modeling, analytical and numerical results, focusing on applications and gaining new insights into the principles of emergence and self-organization.

**Organizer(s) :** Lisa Kreusser, Jan Haskovec

**Classification :** 35B36, 82C22, 70-10, 65M08

**Minisymposium Program :**

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00068 (1/3) : 2D @G501 [Chair: Lisa Maria Kreusser]

## [03562] Emergence of Biological Transportation Networks as a Self-Regulated Process

**Format :** Talk at Waseda University

**Author(s) :** Simone Portaro (KAUST)

**Abstract :** Our purpose is to investigate self-regulating processes modeling biological transportation networks by writing formal  $L^2$ -gradient flow for a tensor valued diffusivity  $D$ . We will explore a broad class of entropy dissipations associated with a purely diffusive model and investigate the formal  $L^2$ -gradient flow of the Fokker-Planck equation. It derives an integral formula for the second variation of the dissipation functional, proving convexity, and couples the Poisson equation for electric potential obtaining the Poisson-Nernst-Planck system. Numerical results are also presented.

## [03929] Bifurcations in collective dynamics: ordered and disordered behaviour

**Format :** Talk at Waseda University

**Author(s) :** Sara Merino-Aceituno (University of Vienna)Raphael Winter (University of Vienna)Christian Schmeiser (University of Vienna)Pierre Degond (University of Toulouse)

**Abstract :** In this talk, I will review some questions that arise around the classical Vicsek model - which is a model for collective dynamics where agents move at a constant speed while trying to adopt the averaged orientation of their neighbours, up to some noise. I will discuss the emergence of bifurcations leading to disordered and ordered motion, depending on the local density of the agents.

This is a very interesting phenomenon: it showcases how two completely different observed behaviours can appear simultaneously from agents that interact following the same rules.

## [04259] A new approach to upscaling of KTEs modelling cell migration

**Format :** Talk at Waseda University

**Author(s) :** Anna Zhigun (Queen's University Belfast)Christina Surulescu (University of Kaiserslautern-Landau)

**Abstract :** A new approach to upscaling of a class of kinetic transport equations that can, e.g. model cell migration in a fibrous environment under the influence of attractants will be presented. It doesn't rely on a Hilbert space setting and provides a unified and transparent way of obtaining both parabolic and hyperbolic scalings. Formal computations are mimicked by rigorous operations with Radon measures. A key tool is a PDE that connects zero and second order moments.

## [04922] Asymptotic limits of transient patterns in a continuous-space interacting particle system.

**Format :** Talk at Waseda University

**Author(s) :** Dietmar B Oelz (University of Queensland)Cecilia Gonzalez Tokman (University of Queensland)

**Abstract :** We study a discrete-time interacting particle system with continuous state space. The process has applications in the modeling of actin filament turnover in biological cells through branching and subsequent rapid debranching. In continuous phase space, it can be interpreted as a voter model and as a step-wise mutation model. Its solutions are characterized by transient clusters reminiscent of either actin filament assemblies in the cell cortex or of the formation of opinion clusters.

We reformulate the process in terms of the inter-particle distances and focus on their marginal and joint distributions. We construct a recurrence relation for the associated characteristic functions and pass to the large population limit reminiscent of the Fleming-Viot super-processes. The precise characterization of all marginal distributions established in this work opens the way to a detailed analysis of cluster dynamics. We also obtain a recurrence relation which enables us to compute the moments of the asymptotic single particle distribution characterizing the transient aggregates. Our results indicate that aggregates have a fat-tailed distribution.

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00068 (2/3) : 2E @G501 [Chair: Jan Haskovec]

## [04504] Model Reduction and Coarse-Graining of Complex Systems

**Format :** Online Talk on Zoom

**Author(s) :** Hong Duong (University of Birmingham)

**Abstract :** Complex systems in nature and in applications (such as molecular systems, crowd dynamics, swarming, opinion formation, just to name a few) are often described by systems of stochastic differential equations (SDEs) and partial differential equations (PDEs). It is often analytically impossible or computationally prohibitively expensive to deal

with the full models due to their high dimensionality (degrees of freedom, number of involved parameters, etc.). It is thus of great importance to approximate such large and complex systems by simpler and lower dimensional ones, while still preserving the essential information from the original model. This procedure is referred to as model reduction or coarse-graining in the literature. In this talk, I will present methods for qualitative and quantitative coarse-graining of several SDEs and PDEs, in the presence or absence of a scale-separation.

## [05047] Splitting methods for optimal control

**Format :** Online Talk on Zoom

**Author(s) :** David Goodwin (Aarhus University)Mohammadali Foroozandeh (Zurich Instruments)Pranav Singh (University of Bath)

**Abstract :** The optimal control of a physical system requires efficient numerical solvers for computing dynamics, accurate gradients, and efficient optimization routines.

Of particular interest in this talk are quantum systems such as spins and electrons under the influence of external time-dependent controls such as lasers and magnetic fields. In this talk I will present a highly efficient optimal control procedure called QOALA which adaptively switches splitting based solvers and utilizes exact gradients.

## [05107] Nonlocal Cross-interaction Systems on Graphs: Energy Landscape and Dynamics

**Format :** Online Talk on Zoom

**Author(s) :** Jan-Frederik Pietschmann (University of Augsburg)Markus Schmidtchen (Technische Universität Dresden)Georg Heinze (University of Augsburg)

**Abstract :** We explore the dynamical behavior and energetic properties of a model of two species that interact nonlocally on finite graphs. We introduce the setting of nonquadratic Finslerian gradient flows on generalized graphs featuring nonlinear mobilities. In a continuous and local setting, this class of systems exhibits a wide variety of patterns, including mixing of the two species, partial engulfment, or phase separation. We showcase how this rich behavior carries over to the graph structure. We present analytical and numerical evidence thereof.

00068 (3/3) : 3C @G501

## [00072] Evolution equations in materials science: Multiscale modeling, analysis, and simulation

**Session Time & Room :**

00072 (1/3) : 3C (Aug.23, 13:20-15:00) @G502

00072 (2/3) : 3D (Aug.23, 15:30-17:10) @G502

00072 (3/3) : 3E (Aug.23, 17:40-19:20) @G502

**Type :** Proposal of Minisymposium

**Abstract :** Materials science has become increasingly efficient and contributes with new products. The increased material functionality relies on good experimental grip on microstructure evolution. Mathematics plays a crucial role in using experimental understanding to shed light where experiments are inaccessible. Mathematical challenges are though unsolved. Elastic porous materials have many practical applications, however the mathematical treatment of elasticity equations for realistic media is underdeveloped as the small-strains-hypothesis needs to be adopted while the porosity of real materials (e. g. when biology is involved) disagrees. Our symposium focuses on the development of advanced mathematical methodologies applicable to materials having complex microstructures.

**Organizer(s) :** Toyohiko Aiki, Adrian Muntean

**Classification :** 35Exx, 74-XX

**Minisymposium Program :**

00072 (1/3) : 3C @G502 [Chair: Toyohiko Aiki]

## [04859] Diffusion in the presence of microstructures: Does vesicle micro-dynamics enhance the signalling among plants macro-transport?

**Format :** Talk at Waseda University

**Author(s) :** Adrian Muntean (Karlstad University)Sander Hille (Leiden University)Omar Richardson (Simula Consulting)

**Abstract :** We study a diffusion-drift problem for signalling among plants in the context of measure-valued equations. We show preliminary results concerning the modelling and mathematical analysis of scenarios involving the macroscopic diffusion of signalling molecules enhanced by a finite number of microvesicles, with own dynamics able to capture and release signals as a relay system. The macro-micro coupling relies on a two-scale transmission condition. Mild solutions will turn to exist and will be positive weak solutions.

## [04217] Morphology formation in ternary mixtures: A continuum model

**Format :** Talk at Waseda University

**Author(s) :** Rainey Lyons (Karlstad University)

**Abstract :** We study the ability of a coupled nonlocal system of two quasilinear parabolic partial differential equations to produce phase separation patterns. This system is derived in the literature as the rigorous hydrodynamic limit of a suitably scaled interacting particle system of Blume–Capel-type driven by Kawasaki dynamics. In this talk, we will discuss the potential of the model to produce morphologies, the growth of these patterns, well-posedness, and regularity of solutions.

## [05044] Homogenisation of an advection–reaction–diffusion process in a porous medium with coupled evolving microstructure

**Format :** Talk at Waseda University

**Author(s) :** Markus Gahn (Heidelberg University)Malte A. Peter (University of Augsburg)Iuliu Sorin Pop (Hasselt University)David Wiedemann (University of Augsburg)

**Abstract :** We consider the homogenization of an advection–reaction–diffusion equation in an evolving porous medium. The microstructure's evolution is coupled with the unknown concentration of a substance, resulting in a free boundary value problem. To rigorously pass to the homogenization limit, we transform the problem into a periodic fixed domain, which results in a highly non-linear problem. We then pass to the homogenization limit.

## [04239] Partial differential equations for moisture transport in porous materials

**Format :** Talk at Waseda University

**Author(s) :** Akiko Morimura (Japan Women's University)Toyohiko Aiki (Japan Women's University)

**Abstract :** We consider the initial-boundary value problems for nonlinear parabolic equations describing moisture transport in a porous material. As a first step in this research, we suppose that the mass distribution in air is given and propose the problem for equation called elliptic-parabolic type. The purpose of this talk is to establish existence and uniqueness of solutions to the approximate problem by applying the evolution equation theory and the standard fixed-point argument.

00072 (2/3) : 3D @G502 [Chair: Adrian Muntean]

## [04230] A two-scale model describing swelling phenomenon in porous materials

**Format :** Talk at Waseda University

**Author(s) :** Kota Kumazaki (Kyoto University of Education)Adrian Muntean (Karlstad University)

**Abstract :** In this talk, we propose a two-scale model describing the swelling phenomenon in porous materials. This model consists of a diffusion equation for the relative humidity distributed in materials and a free boundary problem describing the swelling process in microscopic pores. We consider each microscopic pore as a one-dimensional interval and correspond the interval to each point of materials. In this talk, we discuss the global solvability of this model.

## [04483] Improved corrector regularity in homogenization with non-smooth coefficients

**Format :** Talk at Waseda University

**Author(s) :** Grigor Nika (Karlstad University)

**Abstract :** We propose an advanced model of microscopic heat conduction, capable of addressing size effects in heterogeneous media. By leveraging sound scaling arguments, we enhance the differentiability of the corrector in the classical problem of periodic homogenization of linear elliptic equations in three dimensions. This enables us to elucidate the crucial role that correctors play in quantifying the differences between the microscopic and macroscopic solutions in heterogeneous media. Furthermore, if the data are of the form  $f = \operatorname{div} \mathbf{F}$  with  $\mathbf{F} \in L^3(\Omega, \mathbb{R}^3)$ , then we recover a stronger version of the classical corrector convergence theorem.

## [03965] Solvability of a dynamical model for the elastic curves

**Format :** Talk at Waseda University

**Author(s) :** Chiharu Kosugi (Yamaguchi University) Toyohiko Aiki (Japan Women's University)

**Abstract :** To establish a mathematical model for stretching and shrinking motions of the compressible elastic curves like rubber bands, we discuss problems whose feature is that the strain function is nonlinear and non-smooth, and the stress function has singularity. For the problem, thanks to a priori estimates for the strain from below and center of mass globally in time we can show results on existence, uniqueness, and large time behavior of solutions.

## [04592] Numerical simulations and analysis for mathematical modeling of adsorption phenomena

**Format :** Talk at Waseda University

**Author(s) :** Yusuke Murase (Meijo University)

**Abstract :** In this talk, we discuss numerical simulations and mathematical properties of mathematical modeling for adsorption phenomena and modeling for moisture transport in concrete material. The adsorption model is a free boundary problem composed by heat equation and free boundary equation, and the moisture transport model is combined with adsorption model and diffusion equations. Which is proposed by T. Aiki, K. Kumazaki, N. Sato, and Y. Murase.

00072 (3/3) : 3E @G502 [Chair: Kota Kumazaki]

## [04388] Decay estimates for a unit cell model of composite materials

**Format :** Talk at Waseda University

**Author(s) :** Shuji Yoshikawa (Oita University)

**Abstract :** We shall introduce decay estimates for a unit cell model of composite materials. The model we study here is the one of toy models, but the result corresponds to the first step of a mixture of transmission and waveguide problems from the viewpoint of PDEs.

## [04211] Effective hydromechanic models for fibre-reinforced hydrogels

**Format :** Talk at Waseda University

**Author(s) :** Michael Eden (Karlstad University) Hari Shankar Mahato (IIT Kharagpur)

**Abstract :** We consider highly heterogeneous two-component media composed of a connected fibre-scaffold with periodically distributed inclusions of hydrogel. While the fibres are assumed to be elastic, the hydromechanical response of hydrogel is modeled via Biot's poroelasticity. We show that the resulting mathematical problem admits a unique weak solution and investigate the limit behavior of the solutions with respect to a scale parameter characterizing the heterogeneity of the medium.

## [04680] An elastoplastic model with a time-dependent threshold function

**Format :** Talk at Waseda University

**Author(s) :** Yoshiho Akagawa Takeshi Fukao (Ryukoku University) Risi Kano (Kochi University)

**Abstract :** We investigate the well-posedness of an elastoplastic model described by quasi-variational inequalities, applying the abstract theory of evolution equation. The prototype model is introduced by Duvau-Lions. It is characterized by the constraint for the deviatoric part of the stress tensor. In the case when the constraints depend on time and some unknown strain history, then the model represents more realistic phenomena. This is joint work with Risi Kano (Kochi University), and Takeshi Fukao (Ryukoku University).

# [00082] Development in fractional diffusion equations: models and methods

## Session Time & Room :

00082 (1/3) : 1E (Aug.21, 17:40-19:20) @A618

00082 (2/3) : 4D (Aug.24, 15:30-17:10) @A618

00082 (3/3) : 4E (Aug.24, 17:40-19:20) @A618

## Type :

Proposal of Minisymposium

**Abstract :** The mathematical study of diffusion and its applications has played an important role in modern mathematics. The study of fractional diffusion has become a new trend as a mathematical framework to describe anomalous diffusion. Indeed, in the real world anomalous diffusion is common. We wish to present the last and novel techniques regarding modeling with FDE and its mathematical analysis. In particular we are interested in modeling with the help of FDE, the resulting IBV problems, including free boundary problems. We also pursue the study of the qualitative properties of solutions including self-similar and fundamental solutions.

**Organizer(s) :** Sabrina Roscani, Piotr Rybka

**Classification :** 35R11, 26A33, 80A22

## Minisymposium Program :

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00082 (1/3) : 1E @A618 [Chair: Piotr Rybka]

## [00162] Solution of a fractional Stefan problem using a Landau transformation

### Format :

Talk at Waseda University

### Author(s) :

Vaughan Richard Voller (University of Minnesota)

**Abstract :** The Stefan problem, tracking the motion of a heat conduction driven melt interface, is the classical moving boundary problem. A means of obtaining a solution for such problems is through the use of a variable transformation --- the Landau transformation --- immobilizing the melt interface. Here we apply this technique for the approximate solution of a fractional Stefan problem where the integer time derivative, in the governing diffusion equation, is replaced with a fractional derivative.

## [00166] Fractional diffusion as an intermediate asymptotic regime

### Format :

Talk at Waseda University

### Author(s) :

Gianni Pagnini (BCAM - Basque Center for Applied Mathematics)Paolo Paradisi (ISTI-CNR, Pisa)Silvia Vitali (Eurecat Centre Tecnològic de Catalunya Barcellona )

**Abstract :** A continuous-time random walk driven by two different Markovian hopping-trap mechanisms is investigated and it is shown that paradigmatic features of anomalous diffusion are met. More precisely, anomalous diffusion results from a process that goes through the action of two co-existing Markovian mechanisms acting with different statistical frequency, and the probability of occurrence of this switch between the two Markovian settings originates and fully characterizes the anomalous diffusion. In fact, ensemble and single-particle observables of this model have been studied and they match the main characteristics of anomalous diffusion as they are typically measured in living systems. In particular, the celebrated transition of the walker's distribution from exponential to stretched-exponential and finally to Gaussian distribution is displayed by including also the Brownian yet non-Gaussian interval. Moreover, the model dynamically provides the power-law exponent of the mean-square displacement as a function of the probability of switching between the two Markovian states, namely the fractional order. Hence, fractional diffusion emerges as an intermediate asymptotic regime. Finally, within the present approach, fractional diffusion can be interpreted as a mathematical method for bridging two co-existing equilibrium states in a disordered medium.

This talk is based on: Vitali S, Paradisi P and Pagnini 2022 J. Phys. A: Math. Theor. 55 224012

## [02596] Dissipativity of the energy functional in time-fractional gradient flows

### Format :

Talk at Waseda University

### Author(s) :

Marvin Fritz (Johann Radon Institute for Computational and Applied Mathematics (RICAM))

**Abstract :** In this talk, the monotonicity of the energy functional of time-fractional gradient flows is investigated. It is still unknown whether the energy is dissipating in a timely manner. This characteristic is critical for integer-order gradient flows, and many numerical systems utilize it. We suggest an energy functional that incorporates the solution's part\_1

history, which is reasonable given that time-fractional partial differential equations are nonlocal in time and feature a natural memory effect. On the basis of this new energy, we demonstrate that a time-fractional gradient flow is equivalent to an integer-order flow. In addition, this connection guarantees the dissipative nature of the augmented energy and permits the development of numerical schemes.

00082 (2/3) : 4D @A618 [Chair: Masahiro Yamamoto]

### **[00119] Weak and entropy solutions of time-fractional porous medium type equations**

**Format :** Online Talk on Zoom

**Author(s) :** Petra Wittbold (University of Duisburg-Essen)

**Abstract :** We present results on existence and uniqueness of bounded weak and also unbounded entropy solutions to a degenerate quasilinear subdiffusion problem of porous medium type with bounded measurable diffusion coefficients that may explicitly depend on time. The integro-differential operator in the equation includes, in particular, the time-fractional derivative case.

A key ingredient in the proof of existence is a new compactness criterion of Aubin-Lions type which involves the non-local in time operator.

### **[00167] On different formulations for time-fractional Stefan problems**

**Format :** Online Talk on Zoom

**Author(s) :** Sabrina Roscani (CONICET - Universidad Austral)

**Abstract :** We present a one-dimensional fractional Stefan problem for a memory flux derived from thermodynamic balance statements and provide a memory enthalpy formulation related to the previous model. The Stefan condition for each problem at the free interface is analyzed and numerical simulations obtained from the enthalpy model are given.

### **[00163] Numerical methods for nonlocal and nonlinear parabolic equations with applications in hydrology and climatology**

**Format :** Online Talk on Zoom

**Author(s) :** Lukasz Plociniczak (Wroclaw University of Science and Technology)

**Abstract :** We present some of our results concerning numerical discretizations of nonlinear and fractional in time parabolic equations. Along with a collection of various methods and statements about their convergence and stability, we stress their motivation and real-world applications.

### **[00160] Regularity of weak solutions to parabolic-type problems with distributed order time-fractional derivative**

**Format :** Online Talk on Zoom

**Author(s) :** Katarzyna Ryszewska (Warsaw University of Technology)

**Abstract :** In this talk we will discuss Holder continuity of weak solutions to evolution equations with distributed order time-fractional derivative. It is a generalization of the result for a single order fractional derivative obtained by Prof. Zacher in 2010. The main difficulty to overcome in this case, is the lack of a natural scaling property of the equation.

This is a joint work with Adam Kubica and Prof. Rico Zacher.

00082 (3/3) : 4E @A618 [Chair: Vaughan Richard Voller]

### **[04911] Uniqueness for inverse source problems for time-fractional diffusion-wave equations**

**Format :** Talk at Waseda University

**Author(s) :** Masahiro Yamamoto (The Univ. Tokyo)

**Abstract :** For time-fractional diffusion-wave equations,  $\partial_t^\alpha u(x, t) = -Au + \mu(t)f(x)$  for  $x \in \Omega$ ,  
0

### **[02617] Fractional diffusion equation with psi-Hilfer derivative**

**Format :** Talk at Waseda University

**Author(s) :** M. Manuela Rodrigues (University of Aveiro, Portugal)

**Abstract :** We consider the multidimensional time-fractional diffusion equation with  $\psi$ -Hilfer derivative. An integral representation of the solution to the associated Cauchy problem involving Fox H-functions is obtained. Fractional

moments of arbitrary order are computed. Series representations of the first fundamental solution are presented. Some plots of the fundamental solution are presented for particular choices of the function  $\psi$  and the fractional parameters.

Joint work with N. Vieira (UA - CIDMA), M. Ferreira (IPLeiria~ & ~ CIDMA)

## [02623] On the $\psi$ -Hilfer time-fractional telegraph equation in higher dimensions

**Format :** Talk at Waseda University

**Author(s) :** Nelson Vieira (CIDMA - University of Aveiro)

**Abstract :** We consider the time-fractional telegraph equation in  $\mathbb{R}^n \times \mathbb{R}^+$  with  $\psi$ -Hilfer fractional derivatives. For the solution, we present an integral representation involving Fox H-functions of two variables, and in terms of double series. For  $n = 1$ , we prove the conditions under which we can interpret the first fundamental solution as a probability density function. Some plots of the fundamental solutions are presented. Joint work with M. Ferreira (IPLeiria & CIDMA) and M.M. Rodrigues (CIDMA).

## [02767] The fundamental solution to the space fractional diffusion equation

**Format :** Talk at Waseda University

**Author(s) :** Piotr Rybka (University of Warsaw)Tokinaga Namba (Nippon Steel Corporation)Shoichi Sato (University of Tokyo)

**Abstract :** We consider a one dimensional diffusion equation involving the divergence of the Caputo space derivative of order less than one. We construct a self-similar solution,  $\mathcal{E}$ , which permits us to derive the representation formulas for boundary value problem on the half line. We also present properties of  $\mathcal{E}$ , and we show the infinite speed of signal propagation.

This is a joint research with T.Namaba and S.Sato.

## [00084] Asymptotic approaches to multi-scale PDEs in mathematical physics

**Session Time & Room :**

00084 (1/2) : 5B (Aug.25, 10:40-12:20) @G405

00084 (2/2) : 5C (Aug.25, 13:20-15:00) @G405

**Type :** Proposal of Minisymposium

**Abstract :** Nonlinear PDEs play an important role in modelling many important phenomena observed in physics. One of the main challenges is that the physical problem at hand usually manifests its properties on a hierarchy of scales: the behaviour of the system at the large scale can only be understood by accessing a number of finer scales. Discovering the numerous scales in the governing equations and describing the singularities which appear in asymptotic processes give rise to exciting and difficult research problems (e.g. singular limits in fluid mechanics, macroscopic closures of kinetic models, or incompressible limits for tissue growth models).

**Organizer(s) :** Tomasz Dębiec, Agnieszka Świerczewska-Gwiazda

**Classification :** 35A01, 35B40, 35Q35, 35Q92

**Minisymposium Program :**

00084 (1/2) : 5B @G405 [Chair: Tomasz Dębiec]

## [04992] Relative entropy and application to asymptotic limits for bipolar Euler-Poisson systems.

**Format :** Talk at Waseda University

**Author(s) :** Athanasios Tzavaras (King Abdullah University of Science and Technology (KAUST))Nuno Alves (King Abdullah University of Science and Technology (KAUST))

**Abstract :** The relative entropy method has been a very effective tool for describing asymptotic limit problems in mechanics and mathematical physics. A formalism for Hamiltonian systems can be easily extended to the system of bipolar Euler-Maxwell equations. We will describe here various results on asymptotic limits from bipolar Euler Poisson to

models that are used for the description of plasmas, or (when combined with high-friction limits) to semi-conductors (joint work with Nuno Alves).

## [04461] From compressible euler equation to porous media

**Format :** Talk at Waseda University

**Author(s) :** Piotr Gwiazda (Institute of Mathematics of Polish Academy of Sciences)

**Abstract :** We consider a combined system of Euler, Euler–Korteweg and Euler–Poisson equations. We show the existence of dissipative measure-valued solutions in the cases of repulsive and attractive potential in Euler–Poisson system. Furthermore we show that the strong solutions to the Cahn–Hilliard–Keller–Segel system are a high-friction limit of the dissipative measure-valued solutions to Euler–Korteweg–Poisson equations.

## [03337] On the asymptotic dynamics of point vortices for the lake equations

**Format :** Talk at Waseda University

**Author(s) :** Lars Eric Hientzsch (Bielefeld University)Christophe Lacave (University Grenoble Alpes)Evelyne Miot (University Grenoble Alpes)

**Abstract :** The lake equations describe the evolution of the vertically averaged velocity field of an incompressible inviscid 3D fluid in a domain with spatially varying topography (depth).

We derive the asymptotic dynamics of point vortices for the lake equations with positive depth, when the vorticity is initially sharply concentrated around  $N$  points. More precisely, we show that the vorticity remains concentrated in suitable sense around  $N$  points for all times, and that the trajectories follow the level lines of the depth function.

This is joint work with Christophe Lacave and Evelyne Miot (Université Grenoble Alpes).

## [03190] Strong Convergence of Vorticity in the Viscosity Limit

**Format :** Talk at Waseda University

**Author(s) :** Emil Wiedemann (Universität Erlangen-Nürnberg)

**Abstract :** Consider the 2D incompressible Navier-Stokes equations with initial vorticity in  $L^p$  (\$1

00084 (2/2) : 5C @G405 [Chair: Agnieszka Świerczewska-Gwiazda]

## [05460] Local smooth solvability for the Relativistic Vlasov-Maxwell system.

**Format :** Online Talk on Zoom

**Author(s) :** Slim IBRAHIM (UNIVERSITY OF VICTORIA)Christophe Cheverry (University of Rennes)

**Abstract :** This talk is devoted to the Relativistic Vlasov-Maxwell system in space dimension three. We prove the local smooth solvability for weak topologies (and its long time version for small data). This result is derived from a representation formula decoding how the momentum spreads, and showing that the domain of influence in momentum is controlled by mild information. We do so by developing a Radon Fourier analysis on the RVM system, leading to the study of a class of singular weighted integrals. In the end, we implement our method to construct smooth solutions to the RVM system in the regime of dense, hot and strongly magnetized plasmas. This is done by investigating the stability properties near a class of approximate solutions. This is a joint work with C. Cheverry.

## [04487] Incompressible limit for tumor growth models with convective effects

**Format :** Talk at Waseda University

**Author(s) :** Noemi David (Université de Lyon)Tomasz Dębiec (University of Warsaw)Benoit Perthame (Sorbonne Université)Markus Schmidtchen (Technische Universität Dresden)

**Abstract :** Both compressible and incompressible models have been used in the literature to describe the mechanical aspects of living tissues. Using a stiff pressure law, it is possible to build a bridge between density-based models and free boundary problems where saturation holds. I will present the study of the incompressible limit for advection-porous medium equations and discuss the convergence rate of solutions of the compressible model to solutions of the limit Hele-Shaw problem.

## [03628] Construction of weak solutions to Compressible Navier-Stokes equations

**Format :** Talk at Waseda University

**Author(s) :** Piotr B. Mucha (University of Warsaw)

**Abstract :** We calibrate neural stochastic differential equations jointly to S&P 500 smiles, VIX futures, and VIX smiles. Drifts and volatilities are modeled as neural networks. Minimizing a suitable loss allows us to fit market data for multiple S&P 500 and VIX maturities. A one-factor Markovian stochastic local volatility model is shown to fit both smiles and VIX

futures within bid-ask spreads. The joint calibration actually makes it a pure path-dependent volatility model, confirming the findings in (Guyon, 2022, The VIX Future in Bergomi Models: Fast Approximation Formulas and Joint Calibration with S&P 500 Skew).

## [00085] Singular Problems in Mechanics

### **Session Time & Room :**

00085 (1/3) : 1C (Aug.21, 13:20-15:00) @G406

00085 (2/3) : 1D (Aug.21, 15:30-17:10) @G406

00085 (3/3) : 1E (Aug.21, 17:40-19:20) @G406

### **Type :** Proposal of Minisymposium

**Abstract :** The problem area addresses non-smooth problems stemming from mechanics and described by partial differential equations, inverse and ill-posed problems, non-smooth and nonconvex optimization, optimal control problems, multiscale analysis and homogenization, shape and topology optimization. We focus but are not limited to singularities like cracks, inclusions, aerofoils, defects and inhomogeneities arising in composite structures and multiphase continua, which are governed by systems of variational equations and inequalities. The minisymposium objectives are directed toward sharing advances attained in the mathematical theory, numerical methods, and application of non-smooth problems.

**Organizer(s) :** Victor Kovtunenko, Hiromichi Itou, Alexander Khudnev, Evgeny Rudoy

**Classification :** 35Axx, 49Jxx, 65Kxx, 70Gxx, 76Mxx

### **Minisymposium Program :**

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00085 (1/3) : 1C @G406 [Chair: Hiromichi Itou]

## [00222] Recent progress on the irreversible fracture phase field model

### **Format :** Talk at Waseda University

**Author(s) :** Masato Kimura (Kanazawa University)

**Abstract :** We would like to present our recent progress in the study of the fracture phase field model of the irreversible type. It not only enables us to simulate various kinds of crack propagation phenomena but also realizes a non-healing property and a natural energy gradient structure simultaneously.

## [00267] Fractional Korn inequalities in bounded domains

### **Format :** Talk at Waseda University

**Author(s) :** Davit Harutyunyan (University of California Santa Barbara) Hayk Mikayelyan (University of Nottingham Ningbo China)

### **Abstract :**

The validity of Korn's first inequality in the fractional setting in bounded domains has been open. We resolve this problem by proving that in fact Korn's first inequality holds in the case  $ps > 1$  for fractional  $W_0^{s,p}(\Omega)$  Sobolev fields in open and bounded  $C^1$ -regular domains  $\Omega \subset \mathbb{R}^n$ . Also, in the case  $ps < 1$ , for any open bounded  $C^1$  domain  $\Omega \subset \mathbb{R}^n$  we construct counterexamples to the inequality, i.e., Korn's first inequality fails to hold in bounded domains. The proof of the inequality in the case  $ps > 1$  follows a standard compactness approach adopted in the classical case, combined with a Hardy inequality, and a recently proven Korn second inequality by Mengesha and Scott [\textit{Commun. Math. Sci.}, Vol. 20, No. 2, 405--423, 2022]. The counterexamples constructed in the case  $ps < 1$  are interpolations of a constant affine rigid motion inside the domain away from the boundary, and of the zero field close to the boundary.

## [00266] On Phase Field Approach for Crack Propagation due to Water Pressure in Porous Medium

### **Format :** Talk at Waseda University

**Author(s) :** Sayahdin Alfat (Kanazawa University) Masato Kimura (Kanazawa University)

**Abstract :** The crack propagation in the material due to water pressure was studied. This study involved the poroelasticity theory proposed by M. A. Biot. This study is divided into two parts. In the first part, we derived the poroelasticity theory, and its energy equality and presented several numerical examples. In the second part, we introduce our phase field model with unilateral contact conditions for desiccation cracking by coupling with the Biot model and show energy equality.

## [00171] Asymptotic series solution of variational Stokes problems in planar domain with crack-like singularity

**Format :** Talk at Waseda University

**Author(s) :** Victor Kovtunenko (University of Graz)

**Abstract :** Variational problems for incompressible fluids and solids described by stationary Stokes equations in a planar domain with crack are considered. Based on the Fourier asymptotic analysis, general solutions are derived analytically as power series with respect to the distance to the crack tip. The logarithm terms and angular functions are accounted in the asymptotic expansion using recurrence relations. Boundary conditions of Dirichlet, Neumann, impermeability, non-penetration, and shear at the crack faces determine admissible exponents and parameters in the power series. The principal asymptotic terms are derived in the sector of angle  $2\pi$ , which determine a square-root singularity at the crack tip and presence of log-oscillations of variational solutions for the Stokes problems.

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00085 (2/3) : 1D @G406 [Chair: Victor Kovtunenko]

## [00288] Evolution equations with complete irreversibility

**Format :** Talk at Waseda University

**Author(s) :** Goro Akagi (Tohoku University)

**Abstract :** In this talk, recent developments of studies on evolution equations with complete irreversibility, i.e., solutions are constrained to be monotone in time, will be reviewed. In particular, such evolution equations often arise from fracture and damage mechanics. From mathematical points of view, they are classified as fully nonlinear PDEs, and therefore, it is in general more difficult to prove their well-posedness and reveal dynamics of their solutions. However, by change of variables, they can be rewritten as doubly-nonlinear evolution equations, whose energy and variational structures are available for the analysis. Moreover, they are sometimes equivalently reformulated as semilinear obstacle problems whose obstacle functions coincide with initial data. It will also give us a clue for the analysis. In this talk, we shall overview recent results on diffusion equations and Allen-Cahn equations with complete irreversibility and also some phase-field systems arising from fracture models.

## [00285] $H^2$ -regularity up to boundary for a Bingham fluid model

**Format :** Talk at Waseda University

**Author(s) :** Takahito Kashiwabara (The University of Tokyo)

**Abstract :** Bingham fluid is a model describing the motion of viscoplastic materials. The problem is formulated by a variational inequality, to which weak solvability in the Sobolev space  $H^1$  is well known. However, regularity in  $H^2$  up to the boundary, unlike its interior counterpart, seems to remain open. In this talk, we present such a result for the homogeneous slip boundary value problem, avoiding the difficulty of being unable to get good pressure estimates.

## [00279] On a generalization Kelvin-Voigt model with pressure-dependent moduli

**Format :** Talk at Waseda University

**Author(s) :** Hiromichi Itou (Tokyo University of Science)Victor Kovtunenko (University of Graz)Kumbakonam Rajagopal (Texas A&M University)

**Abstract :** In this talk, we discuss a generalization Kelvin-Voigt model of viscoelasticity whose material moduli depend on the pressure in which both the Cauchy stress and the linearized strain appear linearly. This model is derived from an implicit constitutive relation, and is well-suited to describe porous materials like concrete, ceramics. We show well-posedness for the corresponding variational problem by thresholding the moduli.

## [00287] A reconstruction problem in nanoscale processing by transverse dynamic force microscopy

**Format :** Online Talk on Zoom

**Author(s) :** Alemdar Hasanov Hasanoglu (Kocaeli University)

**Abstract :** In this study, the dynamic model of reconstruction of the shear force in the transverse dynamic force microscopy (TDFM)-cantilever tip-sample interaction is proposed. For this inverse problem, an input-output operator is introduced and then the compactness of this operator, thus, the ill-posedness of the inverse problems is proved. The least square solution of the inverse problem is introduced through the Tikhonov functional. The Lipschitz continuity of the input-output operator is proved. As a consequence of this, the existence of the least square solution is proved. An explicit formula for the Fréchet gradient is derived by making use of the unique solution of the corresponding adjoint problem. This allows us to construct an effective and fast reconstruction algorithm, as the presented computational experiments show.

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00085 (3/3) : 1E @G406 [Chair: Hayk Mikayelyan]

## [00203] On Kirchhoff-Love plates with thin elastic junction

**Format :** Online Talk on Zoom

**Author(s) :** Alexander Khudnev (Lavrentyev Institute of Hydrodynamics of RAS)

**Abstract :** The talk concerns an equilibrium problem for two elastic plates connected by a thin junction (bridge) in a case of Neumann boundary conditions, which provide a non-coercivity for the problem. An existence of solutions is proved. Passages to limits are justified with respect to the rigidity parameter of the junction. In particular, the rigidity parameter tends to infinity and to zero. Limit models are investigated.

## [00235] Optimal Location Problem for Heterogeneous Bodies with Separate and Joined Rigid Inclusions

**Format :** Online Talk on Zoom

**Author(s) :** Niurgun Lazarev (North Eastern Federal University)

**Abstract :** Nonlinear mathematical models describing an equilibrium state of heterogeneous bodies which may come into contact with a fixed non-deformable obstacle are investigated. A possible mechanical interaction of the body and the obstacle is described with the help of the Signorini-type non-penetration condition. We suppose that the heterogeneous bodies consist of an elastic matrix and one or two built-in volume (bulk) rigid inclusions. One of the inclusions can vary its location along a given curve. Considering a location parameter as a control parameter, we formulate an optimal control problem with a cost functional specified by an arbitrary continuous functional on the solution space. Assuming that the location parameter varies in a given closed interval, the solvability of the optimal control problem is established. Furthermore, it is shown that the equilibrium problem for the heterogeneous body with joined two inclusions can be considered as a limiting problem for the family of equilibrium problems for heterogeneous bodies with two separate inclusions.

## [00210] Multiscale analysis of stationary thermoelastic vibrations of a composite material

**Format :** Online Talk on Zoom

**Author(s) :** Evgeny Rudoy (Lavrentyev Institute of Hydrodynamics of the Siberian Branch of the Russian Academy of Sciences)

**Abstract :** The stationary vibrations problem is studied for a planar thermoelastic body incorporating thin inclusions. This problem contains two small positive, which describe the thickness of an individual inclusion and the distance between two neighboring inclusions. Relying on the variational formulation, by means of methods of asymptotic analysis, we investigate the behavior of solutions as parameters tend to zero. We construct models corresponding to limit cases. The work is supported by Russian Scientific Foundation (№ 22-21-00627).

## [00207] An impulsive pseudoparabolic equation with an infinitesimal transition layer

**Format :** Online Talk on Zoom

**Author(s) :** Sergey Alexandrovich Sazhenkov (Altay State University, Barnaul)

**Abstract :** We study the two-dimensional Cauchy problem for the non-instantaneous impulsive pseudoparabolic equation. Such equations arise in filtration theory, thermodynamics, etc. We rigorously justify the passage to the instantaneous impulsive equation and show that, as the duration of the impulse tends to zero, the infinitesimal transition layer is formed, which inherits the profile of the original non-instantaneous impulsive impact. This is a joint work with Dr. Ivan Kuznetsov of the Lavrentyev Institute of Hydrodynamics, Russia.

# [00086] Recent advances in the theory of rogue waves: stability and universality of wave pattern formation

## **Session Time & Room :**

00086 (1/3) : 5B (Aug.25, 10:40-12:20) @G701

00086 (2/3) : 5C (Aug.25, 13:20-15:00) @G701

00086 (3/3) : 5D (Aug.25, 15:30-17:10) @G701

**Type :** Proposal of Minisymposium

**Abstract :** In the last decade, there have been some new developments in the study of rogue-waves of nonlinear integrable evolutionary equations, such as their long-time asymptotics, their stability, their universal patterns, and their onset mechanisms. This minisymposium aims to bring together a group of world-leading researchers to discuss the theoretical, computational, and experimental aspects of this type of extreme wave phenomena.

**Organizer(s) :** Bao-Feng Feng; Peter Miller

**Classification :** 35Q51, 39A36, 35C08

## **Minisymposium Program :**

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00086 (1/3) : 5B @G701 [Chair: Peter Miller]

## [05527] Universal rogue wave patterns and their connections with special polynomials

**Format :** Online Talk on Zoom

**Author(s) :** Jianke Yang (University of Vermont)

**Abstract :** Rogue wave patterns in integrable systems are investigated. We show that universal rogue patterns of various types appear in integrable systems when one of the internal parameters in bilinear expressions of rogue waves gets large, and these universal rogue patterns can be predicted asymptotically by root structures of certain special polynomials, such as the Yablonskii–Vorob’ev polynomial hierarchy and the Okamoto polynomial hierarchies. This is joint work with Dr. Bo Yang of Ningbo University.

## [05532] Determinant formula for Rogue waves and the binomial theorem

**Format :** Talk at Waseda University

**Author(s) :** Yasuhiro Ohta (Kobe University)

**Abstract :** The rogue wave solutions for integrable systems are often given by the determinant formula for tau functions explicitly. The determinant expression is related with the binomial theorem of rational type. We report an observation about the bilinear structure for the tau functions derived through the binomial theorem.

## [05549] Two-dimensional rogue waves generated by resonance collision

**Format :** Online Talk on Zoom

**Author(s) :** Jingsong He (Shenzhen University)

**Abstract :** It is one of important topics to construct rogue waves in two-dimensional integrable systems. In recent years, we have obtained two kinds of rogue wave in few two-dimensional integrable systems by Hirota method. The generating mechanism of them is the resonant collision between different nonlinear waves. In this talk, two kinds of rogue wave of the Davey–Stewartson I equation are discussed with details by analytical and graphic ways. The main results have been published in two papers: Journal of Nonlinear Science 31(2021) 67 and Letters in Mathematical Physics 112(2022)75, co-authored with Jiguang Rao, Athanassios S. Fokas, Yi Cheng.

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00086 (2/3) : 5C @G701 [Chair: Baofeng Feng]

## [04902] Rogue waves of infinite order and their properties, Part 1

**Author(s)** : Deniz Bilman (University of Cincinnati)

**Abstract** : In a study of high-order fundamental rogue wave solutions of the focusing nonlinear Schrödinger equation, a new limiting object termed the rogue wave of infinite order was found in a high-order near-field limit. Subsequently it has been shown that this same limiting object, itself a solution of the focusing nonlinear Schrödinger equation in rescaled variables that also solves differential equations in the Painlevé-III hierarchy, also arises in numerous other settings such as high-order solitons, semiclassical asymptotics, iterated Bäcklund transformations of arbitrary backgrounds, and even other related nonlinear systems. This talk will describe this story and introduce the rogue wave of infinite order and some generalizations of it. This is joint work with Peter D. Miller.

## [04895] Rogue waves of infinite order and their properties, Part 2

**Author(s)** : Peter David Miller (University of Michigan)

**Abstract** : The general rogue wave of infinite order is a family of exact solutions of the focusing nonlinear Schrödinger equation that also solve ordinary differential equations related to Painlevé-III and while being highly-transcendental, nonetheless arise in several natural limits. From their Riemann-Hilbert representation we deduce some elementary properties, detailed asymptotics for large values of the independent variables, and a double-scaling limit. This is joint work with Deniz Bilman.

## [05529] Universality and rogue waves in semi-classical sine-Gordon equation

**Author(s)** : Bingbing Lu (SISSA)Peter David Miller (University of Michigan)

**Abstract** : We study the semiclassical sine-Gordon equation with below threshold pure impulse initial data of Klaus-Shaw type. The system exhibits both phase transition and a gradient catastrophe in finite time. Near the gradient catastrophe point, the asymptotics are universally described by the Painlevé I tritronquée solution away from the poles and the rogue wave solutions of sG near the poles; away from the gradient catastrophe, the phase transition exhibits another type of universality.

## [05518] Large order breathers of the nonlinear Schrödinger equation

**Format** : Talk at Waseda University

**Author(s)** : Xiaoen Zhang (Shandong University of Science and Technology)

**Abstract** : Multi-soliton and high-order soliton solutions are famous in the integrable focusing nonlinear Schrödinger equation. The dynamics of multi-solitons have been well known to us since the 70s of the last century by the determinant analysis. However, there is little progress in the study of high-order solitons. In this work, we would like to analyze the large-order asymptotics for the high-order breathers, which are special cases of double high-order solitons with the same velocity. To analyze the large order dynamics, we first convert the representation of Darboux transformation into a framework of the Riemann-Hilbert problem. Then we show that there exist five distinct asymptotic regions by the Deift-Zhou nonlinear steepest descent method. More importantly, we first find a novel genus-three asymptotic region, which uncovers that the maximal genus is connected with the number of spectral parameters. All results of the asymptotic analysis are verified by the numerical method.

00086 (3/3) : 5D @G701 [Chair: Y. Ohta]

## [04536] On stability of KdV solitons

**Format** : Talk at Waseda University

**Author(s)** : Derchyi Wu (Institute of Mathematics, Academia Sinica,)

**Abstract** : Applying the inverse scattering theory, we present an orbital stability theorem of KdV  $n$ -solitons with explicit phase shifts.

## [05530] Rogue waves in the massive Thirring model

**Format** : Online Talk on Zoom

**Author(s)** : Junchao Chen (Lishui University)

**Abstract** : In this talk, I will talk about general rogue wave solutions in the massive Thirring (MT) model. These rational solutions are derived by using the KP hierarchy reduction method and presented explicitly in terms of determinants whose matrix elements are elementary Schur polynomials. In the reduction process, three reduction conditions including one index- and two dimension-ones are proved to be consistent by only one constraint relation on parameters of tau-functions of the KP-Toda hierarchy. It is found that the rogue wave solutions in the MT model depend on two background parameters, which influence their orientation and duration. Differing from many other coupled integrable systems, the MT model only admits the rogue waves of bright-type, and the higher-order rogue waves represent the superposition of fundamental ones in which the non-reducible parameters determine the arrangement patterns of

fundamental rogue waves. Particularly, the super rogue wave at each order can be achieved simply by setting all internal parameters to be zero, resulting in the amplitude of the sole huge peak of order  $N$  being  $2N + 1$  times the background. Finally, rogue wave patterns are discussed when one of the internal parameters is large. Similar to other integrable equations, the patterns are shown to be associated with the root structures of the Yablonskii-Vorob'ev polynomial hierarchy through a linear transformation. This work is joint with Bo Yang and Bao-Feng Feng.

### [03606] Resonant breather and rogue wave solutions to a coupled Sasa-Satsuma equation

**Format :** Talk at Waseda University

**Author(s) :** Baofeng Feng (University of Texas Rio Grande Valley )Chengfa Wu (Shenzhen University)

**Abstract :** We firstly derive a set of 7 bilinear equations for a coupled Sasa-Satsuma (CSSI) equation under nonzero boundary conditions and show that they can be reduced from the discrete and continuous KP-Toda hierarchy through a series of reductions such as the CKP-, dimension- and complex conjugate reductions. Then, we derive breather and rogue wave solutions in determinant form. In the last, we show the dynamical behavior of these solutions especially resonant breather solutions.

### [03607] Resonant breather and rogue wave solutions to a coupled Sasa-Satsuma equation

**Author(s) :** Baofeng Feng (University of Texas Rio Grande Valley )Chengfa Wu (Shenzhen University)

**Abstract :** We firstly derive a set of 7 bilinear equations for a coupled Sasa-Satsuma (CSSI) equation under nonzero boundary conditions and show they can be reduced from the discrete and continuous KP-Toda hierarchy through a series of reductions such as CKP-, dimension- and complex conjugate reductions. Then, we derive breather and rogue wave solutions in determinant form. In the last, we show the dynamical behavior of these solutions especially resonant breather solutions.

## [00087] Intersection of Machine Learning, Dynamical Systems and Control

**Session Time & Room :**

00087 (1/2) : 2C (Aug.22, 13:20-15:00) @A615

00087 (2/2) : 2D (Aug.22, 15:30-17:10) @A615

**Type :** Proposal of Minisymposium

**Abstract :** In recent years, the intersection of machine learning, dynamical systems and control has created some new excitement in different disciplines. On the one hand, machine learning-based algorithms have opened up new opportunities in studying dynamical systems and control problems, particularly in high dimensions. On the other hand, the controlled dynamical system perspective of deep learning has also brought new insight in machine learning. This minisymposium will bring together experts in different areas to explore these new exciting opportunities. The goal is to stimulate researchers from different communities to think rigorously across disciplines and move toward new questions.

**Organizer(s) :** Jiequn Han, Qianxiao Li, Xiang Zhou

**Classification :** 65Lxx, 65Mxx, 49Mxx, 68T07, Machine Learning, Dynamical Systems, Control Theory

**Minisymposium Program :**

00087 (1/2) : 2C @A615 [Chair: Jiequn Han]

### [02826] Solving Parametric PDEs by Deep Learning

**Format :** Talk at Waseda University

**Author(s) :** Bin Dong (Peking University)

**Abstract :** Deep learning continues to dominate machine learning and has been successful in computer vision, natural language processing, etc. Its impact has now expanded to many research areas in science and engineering. In this talk, I will present a series of our recent works on combining wisdom from traditional numerical PDE methods and machine learning to design data-driven solvers for parametric PDEs and their applications in fluid simulations. This is joint work with Professor Jinchao Xu, my previous Ph.D. student Yuyan Chen, and my colleagues from Huawei MindSpore AI + Scientific Computing team and the Shanghai Aircraft Design and Research Institute of The Commercial Aircraft Corporation of China.

## [02805] Training Deep ResNet with Batch Normalization as a First-order Mean Field Type Problem

**Format :** Talk at Waseda University

**Author(s) :** Phillip Sheung Chi Yam (Department of Statistics, Chinese University of Hong Kong)

**Abstract :** In this talk, we shall discuss a numerical scheme for training Deep Residual Networks that incorporates the popular Batch Normalization technique into the recently proposed extended Method of Successive Approximation in the work of Li, Chen, Tai and E, The Journal of Machine Learning Research (2017), 18: 5998–6026, and its effectiveness has been demonstrated by numerical studies. The convergence of this proposed scheme depends on the first-order mean field theory, namely the resolution of the corresponding generic first-order mean field type problems inherited from the augmented Hamiltonian, and we shall introduce this brand-new fundamental theory behind.

## [02933] Dynamics-Quantified Implicit Biases of Large Learning Rates

**Format :** Talk at Waseda University

**Author(s) :** Molei Tao (Georgia Institute of Technology)

**Abstract :** This talk will describe some nontrivial (and pleasant) effects of large learning rates, which are often used in machine learning practice but defy traditional optimization theory. I will first show how large learning rates can lead to quantitative escapes from local minima, via chaos, which is an alternative mechanism to commonly known noisy escapes due to stochastic gradients. I will then report how large learning rates provably bias toward flatter minimizers, which arguably generalize better.

## [04799] An optimal control perspective on diffusion-based generative modeling leading to robust numerical methods

**Format :** Talk at Waseda University

**Author(s) :** Lorenz Richter (Zuse Institute Berlin, dida)

**Abstract :** This talk establishes a connection between generative modeling based on SDEs and three classical fields of mathematics, namely stochastic optimal control, PDEs and path space measures. Those perspectives will be both of theoretical and practical value, for instance allowing to transfer methods from one to the respective other field or leading to novel algorithms for sampling from unnormalized densities. Further, the connection to HJB equations leads to novel loss functions which exhibit favorable statistical properties and result in improved convergence of respective algorithms.

00087 (2/2) : 2D @A615 [Chair: Qianxiao Li]

## [04826] Learning high-dimensional feedback laws for collective dynamics control

**Format :** Talk at Waseda University

**Author(s) :** Dante Kalise (Imperial College London)Giacomo Albi (University of Verona)Sara Bicego (Imperial College London)

**Abstract :** We discuss the control of collective dynamics for an ensemble of high-dimensional particles. The collective behaviour of the system is modelled using a kinetic approach, reducing the problem to efficiently sampling binary interactions between controlled agents. However, as individual agents are high-dimensional themselves, the controlled binary interactions correspond to large-scale dynamic programming problems, for which we propose a supervised learning approach based on discrete-time State-dependent Riccati Equations and recurrent neural networks.

## [05378] Sparse Kernel Flows for Learning 132 Chaotic Dynamical Systems from Data

**Format :** Talk at Waseda University

**Author(s) :** Boumediene Hamzi (Caltech)Lu Yang (Nanjing University of Aeronautics and Astronautics)Xiuwen Sun (Nanjing University of Aeronautics and Astronautics)Houman Owhadi (California Institute of Technology)Naiping Xie (NUAA)

**Abstract :** Regressing the vector field of a dynamical system from a finite number of observed states is a natural way to learn surrogate models for such systems. As shown in previous work, a simple and interpretable way to learn a dynamical system from data is to interpolate its vector-field with a data-adapted kernel which can be learned by using Kernel Flows.

The method of Kernel Flows is a trainable machine learning method that learns the optimal parameters of a kernel based on the premise that a kernel is good if there is no significant loss in accuracy if half of the data is used. The objective function could be a short-term prediction or some other objective. However, this

method is limited by the choice of the base kernel.

In this paper, we introduce the method of Sparse Kernel Flows in order to learn the “best” kernel by starting from a large dictionary of kernels. It is based on sparsifying a kernel that is a linear combination of elemental kernels. We apply this approach to a library of 132 chaotic systems. Presentation based on <https://arxiv.org/pdf/2301.10321.pdf>

## [05395] Distributed Control of Partial Differential Equations Using Convolutional Reinforcement Learning

**Format :** Talk at Waseda University

**Author(s) :** Sebastian Peitz (Universität Paderborn)Jan Stenner (Universität Paderborn)Vikas Chidananda (Universität Paderborn)Steven Brunton (UW)Kunihiro Taira (UCLA)

**Abstract :** We present a convolutional framework which significantly reduces the complexity and thus, the computational effort for distributed reinforcement learning control of partial differential equations (PDEs). Exploiting translational invariances, the high-dimensional distributed control problem can be transformed into a multi-agent control problem with many identical agents. Furthermore, using the fact that information is transported with finite velocity in many cases, the dimension of the agents’ environment can be drastically reduced using a convolution operation over the state space of the PDE. In this setting, the complexity can be flexibly adjusted via the kernel width or using a stride greater than one. A central question in this framework is the definition of the reward function, which may consist of both local and global contributions. We demonstrate the performance of the proposed framework using several standard PDE examples with increasing complexity, where stabilization is achieved by training a low-dimensional DDPG agent with small training effort.

## [00088] Machine learning in infinite dimensions

**Session Time & Room :**

00088 (1/3) : 4C (Aug.24, 13:20-15:00) @F311

00088 (2/3) : 4D (Aug.24, 15:30-17:10) @F311

00088 (3/3) : 4E (Aug.24, 17:40-19:20) @F311

**Type :** Proposal of Minisymposium

**Abstract :** Lifting high-dimensional problems to an infinite-dimensional space and designing algorithms in that setting has been a fruitful idea in many areas of applied mathematics, including inverse problems, optimisation, and partial differential equations. This approach is sometimes referred to as “optimise-then-discretise” and allows one to develop algorithms that are inherently dimension- and discretisation-independent and typically perform better in high-dimensional problems. In the context of machine learning, this approach has gained significant attention in the context of operator learning. This workshop explores approaches that involve the approximation of functions with values in an infinite-dimensional space and their connections to partial differential equations.

**Organizer(s) :** Bamdad Hosseini, Yury Korolev, Jonas Latz

**Classification :** 46E40, 68T07, 62H30, Operator learning, representer theorems, PDE learning, vector-valued neural networks

**Minisymposium Program :**

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00088 (1/3) : 4C @F311 [Chair: Yury Korolev]

## [02760] Approximation by structured deep neural networks

**Format :** Talk at Waseda University

**Author(s) :** Dingxuan Zhou (University of Sydney)

**Abstract :** Deep learning based on deep neural networks possessing network architectures has been powerful in practical applications but is less understood theoretically. Structured neural networks are particularly difficult to analyze. An important family of structured neural networks is deep convolutional neural networks possessing convolutional structures. The convolutional architecture is key for the computational efficiency but raises scientific challenges. We describe a mathematical theory of approximating and learning functions or operators by structured deep neural networks.

## [03794] Learning High-Dimensional Banach-Valued Functions from Limited Data with Deep Neural Networks

**Format :** Talk at Waseda University

**Author(s) :** Nick Dexter (Florida State University) Ben Adcock (Simon Fraser University) Sebastian Moraga (Simon Fraser University) Simone Brugiapaglia (Concordia University)

**Abstract :** Reconstructing high-dimensional functions from few samples is important for uncertainty quantification in computational science. Deep learning has achieved impressive results in parameterized PDE problems with solutions in Hilbert or Banach spaces. This work proposes a novel algorithmic approach using DL, compressed sensing, orthogonal polynomials, and finite elements to approximate smooth functions in infinite-dimensional Banach spaces. Theoretical analysis provides explicit guarantees on error and sample complexity, and numerical experiments demonstrate accurate approximations on challenging benchmark problems.

## [04519] Kernel methods for learning operators between infinite dimensional Banach spaces

**Format :** Talk at Waseda University

**Author(s) :** Pau Batlle (California Institute of Technology) Matthieu Darcy (California Institute of Technology) Houman Owhadi (California Institute of Technology) Bamdad Hosseini (University of Washington)

**Abstract :** We introduce a kernel-based framework for learning operators between Banach spaces. We show that even with simple kernels, our approach is competitive in terms of cost-accuracy trade-off and either matches or beats the performance of NN methods on a majority of PDE-based benchmarks. Additionally, our framework offers several advantages inherited from kernel methods: simplicity, interpretability, convergence guarantees, a priori error estimates, and Bayesian UQ. It is therefore a natural benchmark for operator learning problems.

## [03223] A duality framework for generalization analysis of random feature models and two-layer neural networks

**Format :** Talk at Waseda University

**Author(s) :** Hongrui Chen (Peking University) Jihao Long (Princeton University) Lei Wu (Peking University)

**Abstract :** We consider the problem of learning functions in the  $\mathcal{F}_{p,\pi}$  and Barron spaces, which are natural function spaces that arise in the high-dimensional analysis of random feature models (RFMs) and two-layer neural networks. Through a duality analysis, we reveal that the approximation and estimation of these spaces can be considered equivalent in a certain sense. This enables us to focus on the easier problem of approximation and estimation when studying the generalization of both models. The dual equivalence is established by defining an information-based complexity that can effectively control estimation errors. Additionally, we demonstrate the flexibility of our duality framework through comprehensive analyses of two concrete applications.

The first application is to study learning functions in  $\mathcal{F}_{p,\pi}$  with RFMs. We prove that the learning does not suffer from the curse of dimensionality as long as  $p > 1$ , implying RFMs can work beyond the kernel regime. Our analysis extends existing results (Celentano et al., 2021) to the noisy case and removes the requirement of overparameterization.

The second application is to investigate the learnability of reproducing kernel Hilbert space (RKHS) under the uniform metric. We derive both lower and upper bounds of the minimax estimation error by using the spectrum of the associated kernel. We then apply these bounds to dot-product kernels and analyze how they scale with the input dimension. Our results suggest that learning with ReLU (random) features is generally intractable in terms of reaching high uniform accuracy.

00088 (2/3) : 4D @F311 [Chair: Bamdad Hosseini]

## [03216] Reliable extrapolation of deep neural operators informed by physics or sparse observations

**Author(s) :** Lu Lu (University of Pennsylvania) Min Zhu (University of Pennsylvania)

**Abstract :** Deep neural operators can learn nonlinear mappings between infinite-dimensional function spaces via deep neural networks. As promising surrogate solvers of partial differential equations (PDEs) for real-time prediction, deep neural operators such as deep operator networks (DeepONets) provide a new simulation paradigm in science and engineering. Pure data-driven neural operators and deep learning models, in general, are usually limited to interpolation scenarios, where new predictions utilize inputs within the support of the training set. However, in the inference stage of real-world applications, the input may lie outside the support, i.e., extrapolation is required, which may result to large errors and unavoidable failure of deep learning models. Here, we address this challenge of extrapolation for deep neural operators. First, we systematically investigate the extrapolation behavior of DeepONets by quantifying the extrapolation complexity via the 2-Wasserstein distance between two function spaces and propose a new behavior of bias-variance trade-off for extrapolation with respect to model capacity. Subsequently, we develop a complete workflow, including

extrapolation determination, and we propose five reliable learning methods that guarantee a safe prediction under extrapolation by requiring additional information -- the governing PDEs of the system or sparse new observations. The proposed methods are based on either fine-tuning a pre-trained DeepONet or multifidelity learning. We demonstrate the effectiveness of the proposed framework for various types of parametric PDEs. Our systematic comparisons provide practical guidelines for selecting a proper extrapolation method depending on the available information, desired accuracy, and required inference speed.

## [04824] Analysis of Neural Networks : Blessings of Width, Curses of Depth

**Format :** Online Talk on Zoom

**Author(s) :** Lénaïc Chizat (EPFL)

**Abstract :** I will present several results around the large-width limit of gradient-based algorithms for artificial neural networks (NNs). After a review of two-layer NNs, I will discuss the case of deep NNs where the non-linear dynamics that arises turns out much less tractable, because of how the random matrices of the initialization interact. I will finally elaborate on the case of deep linear NNs where we have obtained a complete description of the dynamics.

## [02466] Mirror Descent with Relative Smoothness in Measure Spaces, with application to Sinkhorn and EM

**Format :** Talk at Waseda University

**Author(s) :** Anna Korba (ENSAE/CREST)Pierre-Cyril Aubin-Frankowski (INRIA/Ecole Normale Supérieure)Flavien Léger (INRIA)

**Abstract :** Many problems in machine learning can be formulated as optimizing a convex functional over a vector space of measures. This paper studies the convergence of the mirror descent algorithm in this infinite-dimensional setting. Defining Bregman divergences through directional derivatives, we derive the convergence of the scheme for relatively smooth and convex pairs of functionals. Such assumptions allow to handle non-smooth functionals such as the Kullback–Leibler (KL) divergence. Applying our result to joint distributions and KL, we show that Sinkhorn’s primal iterations for entropic optimal transport in the continuous setting correspond to a mirror descent, and we obtain a new proof of its (sub)linear convergence. We also show that Expectation Maximization (EM) can always formally be written as a mirror descent. When optimizing only on the latent distribution while fixing the mixtures parameters – which corresponds to the Richardson–Lucy deconvolution scheme in signal processing – we derive sublinear rates of convergence.

## [05291] Covariance-Modulated Optimal Transport Geometry

**Format :** Talk at Waseda University

**Author(s) :** Franca Hoffmann (California Institute of Technology)André Schlichting (University of Münster)Martin Burger (DESY and University of Hamburg)Daniel Matthes (Technische Universität München)Matthias Erbar (Universität Bielefeld)

**Abstract :** We present a variant of the dynamical optimal transport problem in which the energy to be minimised is modulated by the covariance matrix of the current distribution. Such transport metrics arise naturally in mean-field limits of certain ensemble Kalman methods for solving inverse problems. We show that the transport problem splits into two coupled minimization problems up to degrees of freedom given by rotations: one for the evolution of mean and covariance of the interpolating curve, and one for its shape. Similarly, on the level of the gradient flows a similar splitting into the evolution of moments and shapes of the distribution can be observed. Those show better convergence properties in comparison to the classical Wasserstein metric in terms of exponential convergence rates independent of the Gaussian target.

00088 (3/3) : 4E @F311 [Chair: Bamdad Hosseini]

## [04018] Learning PDE operators with neural networks

**Format :** Talk at Waseda University

**Author(s) :** Elizabeth Qian (Georgia Institute of Technology)

**Abstract :** The term ‘surrogate modeling’ in computational science and engineering refers to the development of computationally efficient approximations for expensive simulations such as those arising from numerical solution of partial differential equations (PDEs). Surrogate modeling is an enabling methodology for many-query computations in science and engineering which include iterative methods in optimization and sampling methods in uncertainty quantification. Over the last few years several approaches to surrogate modeling for PDEs using neural networks have emerged motivated by successes in using neural networks to approximate nonlinear maps in other areas. In principle the relative merits of these different approaches can be evaluated by understanding for each one the cost required to achieve a given level of accuracy. However the absence of a complete theory of approximation error for these approaches makes

it difficult to assess this cost-accuracy trade-off. In this talk we provide a careful numerical study of this issue comparing a variety of different neural network architectures for operator approximation across a range of problems arising from PDE models in continuum mechanics.

### [04864] Learning solution operators for PDEs with uncertainty

**Format :** Talk at Waseda University

**Author(s) :** Emilia Magnani (University of Tübingen)Nicholas Krämer (University of Tübingen)Runa Eschenhagen (University of Cambridge)Philipp Hennig (University of Tübingen)Lorenzo Rosasco (University of Genova & MIT)

**Abstract :** We provide a Bayesian formulation of the problem of learning solution operators of PDEs in the formalism of Gaussian processes. We extend this treatment to recent deep architectures (neural operators) that have shown promising results to tackle this task. We provide them with uncertainty estimates through methods from Bayesian deep learning. Finally, we consider particular types of operators (convolutions) and investigate the process of learning these in the context of functional regression in inverse problems.

### [04774] Unsupervised Learning of the Total Variation Flow

**Format :** Talk at Waseda University

**Author(s) :** Tamara G Grossmann (University of Cambridge)Sören Dittmer (University of Cambridge)Yury Korolev (University of Bath)Carola-Bibiane Schönlieb (University of Cambridge)

**Abstract :** The total variation (TV) flow generates a scale-space representation of an image based on the TV functional. This gradientflow observes desirable features for images and enables texture analysis. The standard numerical approach requires solving multiple non-smooth optimisation problems, this is often prohibitively expensive. We propose the TVflowNET, a neural network approach to compute the solution. We significantly speed up the computation time and show that the TVflowNET approximates the TV flow solution with high fidelity.

### [03051] On solving/learning nonlinear PDEs with GPs

**Format :** Talk at Waseda University

**Author(s) :** Houman Owhadi (California Institute of Technology)

**Abstract :** We present a simple, rigorous, and unified framework for solving and learning arbitrary nonlinear PDEs with GPs. The proposed approach inherits the error bounds of kernel interpolation methods and the near-linear complexity of linear solvers for dense kernel matrices. Its generalization to high-dimensional PDEs comes with error bounds exhibiting a tradeoff between dimensionality and regularity. Parts of this talk are joint work with Pau Batlle Franch, Yifan Chen, Bamdad Hosseini, Florian Schäfer, and Andrew Stuart.

## [00090] Recent advances in the theory of rogue waves: one- and multi-component models in 1+1 and 2+1 dimensions

**Session Time & Room :**

00090 (1/3) : 1C (Aug.21, 13:20-15:00) @G801

00090 (2/3) : 1D (Aug.21, 15:30-17:10) @G801

00090 (3/3) : 1E (Aug.21, 17:40-19:20) @G801

**Type :** Proposal of Minisymposium

**Abstract :** Recent advances in the theory of nonlinear waves have allowed a better understanding of the underlying mechanisms leading to the formation of space-time localised extreme waves, often referred in the literature as rogue waves, in systems modelled by nonlinear PDEs of integrable and non-integrable type. Many theoretical questions remain open as for a qualitative and quantitative description of the evolution of a localised or periodic perturbation on a given background. The aim of this minisymposium is to gather world-leading experts in the field to discuss the most recent results about the onset and recurrence of rogue waves in nonlinear media.

**Organizer(s) :** Prof Sara Lombardo (Heriot-Watt University, UK), Dr Matteo Sommacal (Northumbria University, UK)

**Classification :** 35Qxx, 35C08, 37K10, 76B15, 76E30, Nonlinear waves, Rational solutions, Rogue waves, Integrability, Stability

**Minisymposium Program :**

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00090 (1/3) : 1C @G801 [Chair: Matteo Sommacal]

part\_1

## [03779] Maximal Amplitudes of N-Phase Solutions of a Modified NLS Equation

**Format :** Online Talk on Zoom

**Author(s) :** Otis Wright (Cedarville University)

**Abstract :** An effective method for finding the maximal amplitudes of N-phase solutions of a modified nonlinear Schrödinger equation is discussed.

## [05214] The effects of damping on rogue wave formation and permanent downshifting

**Format :** Online Talk on Zoom

**Author(s) :** Cosntance Schober (University of Central Florida)Annalisa Maria Calini (College of Charleston )

**Abstract :** The effects of damping on the B-F instability, rogue wave formation, and permanent downshifting are discussed

in the framework of the viscous damped

higher order nonlinear Schrodinger (v-HONLS) equation. The linear stability analysis of the damped Stokes wave solution is presented.

Numerical simulations of the v-HONLS with unstable Stokes wave initial data indicate the inclusion of viscosity enables permanent downshifting and rogue waves typically do not develop after the time of permanent downshift.

## [04450] Rogue-wave formation scenarios for focusing NLS with parabolic initial data

**Format :** Talk at Waseda University

**Author(s) :** Francesco Demontis (University of Cagliari)Giovanni Ortenzi (University of Torino)Giacomo Roberti (Northumbria University)Matteo Sommacal (Northumbria University)

**Abstract :** We study focussing NLS for compactly-supported parabolic initial data with constant chirp. In the absence of dispersion, we provide a criterion for blow-up, generalising a result by Talanov et al. In the presence of dispersion, the same criterion determines, even beyond the semi-classical regime, the formation of rogue-waves, whose onset time is predicted by the corresponding dispersionless catastrophe time. Numerics suggest that the chirp controls the prevailing scenario among two competing mechanisms for rogue-wave formation.

## [04494] Stability of plane waves for the Yajima-Oikawa-Newell equation

**Format :** Talk at Waseda University

**Author(s) :** Marcos Caso-Huerta (Northumbria University)

**Abstract :** A new, integrable long wave-short wave model is proposed, encompassing Yajima-Oikawa and Newell systems as particular choices of the coefficients. The stability of its plane waves is studied in an algebraic-geometric approach making use of its Lax pair. The stability spectra are explicitly computed, leading to identifying a relation between the topology of the spectra and the gain of the system. This allows one to predict regions of existence for rogue wave type solutions.

00090 (2/3) : 1D @G801 [Chair: Sara Lombardo]

## [04830] Rogue waves in 1+1 and in 2+1 dimensions

**Format :** Online Talk on Zoom

**Author(s) :** Paolo Maria Santini (Dept. of Physics, University "La Sapienza")Petr Grinevich (Steklov Math. Institute, Moscow)Francesco Coppini (Dept. of Physics, University "La Sapienza")

**Abstract :** We summarize recent results on the theory of rogue waves. 1) Relevant exact rogue wave (RW) solutions of integrable continuous, discrete, and relativistic NLS type field theories in 1+1 and/or 2+1 dimensions. 2) Analytic description of the recurrence of RWs. 3) Stability properties of exact RW solutions. 4) The effect of perturbations of the model on the RW dynamics.

## [04499] Finite-gap approach to the Davey-Stewardson-2 rogue waves

**Format :** Online Talk on Zoom

**Author(s) :** Petr G. Grinevich (Steklov Mathematical Institute, RAS)Paolo Maria Santini (University Roma-1 "La Sapienza", INFT)

**Abstract :** In a recent series of paper we showed that for the 1+1 dimensional soliton systems the finite-gap formulas for solutions describing the generation of rogue waves can be essentially simplified in the leading order. The origin of this

simplification is that the Cauchy problem for rogue waves naturally contains a small parameter therefore the spectral curve is a small perturbation of a rational one.

We show that this approach can be naturally extended to the focusing Davey-Stewartson 2 equation, which is 2+1 integrable model admitting rogue waves type solutions. Again, in the leading order we obtain elementary formulas for the rogue waves Cauchy problem.

## [04876] Non-commutative soliton equations: some solutions of matrix mKdV equation

**Format :** Online Talk on Zoom

**Author(s) :** Sandra Carillo (Dip SBAI, SAPIENZA UNIV. & INFN, Sez. IV, MMNLP)Cornelia Schiebold (Sundswall University)

**Abstract :** Solutions of matrix mKdV equation are presented. They can be termed soliton solutions since they exhibit the typical behaviour of solitons. The asymptotics of 2-soliton solutions of the d x d-matrix modified Korteweg de-Vries equation is given under the assumption that the involved spectral matrices are invertible. This work is motivated by explicit solutions by the authors, and bases on an explicit solution formula for the N-soliton solutions previously obtained.

## [05198] Spectral approaches to wave instability

**Format :** Talk at Waseda University

**Author(s) :** Sara Lombardo (Heriot-Watt University)

**Abstract :** Recent spectral techniques to study the stability of nonlinear waves will be reviewed in connection with more established results, with a particular focus on the case of nonlinear evolution equations of integrable type.

00090 (3/3) : 1E @G801

## [00107] Randomized numerical linear algebra

**Session Time & Room :**

00107 (1/3) : 4C (Aug.24, 13:20-15:00) @E603

00107 (2/3) : 4D (Aug.24, 15:30-17:10) @E603

00107 (3/3) : 4E (Aug.24, 17:40-19:20) @E603

**Type :** Proposal of Minisymposium

**Abstract :** Randomized numerical linear algebra (RNLA) is an emerging field of computational mathematics that has enabled matrix computations of unprecedented scale. Given the increasing size of data sets, RNLA is often the only way to reasonably perform computations. In addition to speed, RNLA provides solutions with exceptional accuracy and robustness. Success stories in RNLA include low-rank approximation, least-squares problems, and trace estimation. In addition, the field has witnessed recent progress in linear systems, eigenvalue problems, and tensor approximation. This minisymposium aims to bring together researchers working in RNLA to present recent progress, discuss challenges, and share ideas.

**Organizer(s) :** Ethan Epperly, Per-Gunnar Martinsson, Yuji Nakatsukasa, Robert Webber  
**Sponsor :** This session is sponsored by the SIAM Activity Group on Computational Science and Engineering.

**Classification :** 65F55, 65C99, 68T09

**Minisymposium Program :**

00107 (1/3) : 4C @E603 [Chair: Ethan Epperly]

## [03344] Randomized low-rank approximation: Where we've been and where we're going

**Format :** Talk at Waseda University

**Author(s) :** Robert Webber (California Institute of Technology)

**Abstract :** I will survey randomized algorithms for low-rank matrix approximation. These algorithms are helpful for speeding up computations involving high-dimensional matrices. When the singular values of the target matrix decay quickly, the most efficient low-rank approximation algorithms are "randomized SVD" and, if the matrix is positive semidefinite, "randomized Nyström". When the singular values of the target matrix decay slowly, low-rank approximation becomes more difficult and the best-performing algorithms are instead randomized block Krylov methods.

## [04049] Efficient Bounds for Canonical Angles in Randomized Subspace Approximations

**Format :** Online Talk on Zoom

**Author(s) :** Yijun Dong (UT Austin)Per-Gunnar Martinsson (UT Austin)Yuji Nakatsukasa (University of Oxford)

**Abstract :** Randomized subspace approximation is an effective approach for approximating partial SVDs of large matrices, whose accuracy has been extensively analyzed in terms of residual errors. However, our understanding of the computed singular subspaces remains limited. We present bounds and estimates for canonical angles of randomized subspace approximation that can be computed efficiently either a priori or a posteriori. Numerical experiments demonstrate the empirical effectiveness of these canonical angle approximations under various algorithmic choices.

## [03767] Randomized Nyström approximation for symmetric indefinite matrices

**Format :** Talk at Waseda University

**Author(s) :** Taejun Park (University of Oxford)Yuji Nakatsukasa (University of Oxford)

**Abstract :** In this talk, we present a variant of the Nyström method for symmetric indefinite matrices. The Nyström method is a popular choice for symmetric positive semi-definite matrices. However, the method can fail when the matrix is indefinite, for which the error can be large. We first identify the main challenges in finding a robust Nyström approximation to symmetric indefinite matrices and describe an algorithm, whose robustness for symmetric indefinite matrices is illustrated with experiments.

## [04567] The Cluster and the Gap in Randomized Subspace Iteration

**Format :** Talk at Waseda University

**Author(s) :** Eric Hallman (Google)

**Abstract :** This talk concerns the convergence rates of the singular values and vectors when running randomized subspace iteration. Its aim is to present a single clean approach (based on the techniques of (Yuan/Gu/Li, 2018)) that can be used to derive a variety of existing bounds in the literature, both gap-dependent and gap-independent. Limitations of the proof strategy are discussed, as well as its extensions to randomized block Lanczos.

00107 (2/3) : 4D @E603 [Chair: Per-Gunnar Martinsson]

## [04958] RandNLA for Faster Convex Optimization

**Format :** Talk at Waseda University

**Author(s) :** Zachary Frangella (Stanford University)

**Abstract :** In this talk, we show how to accelerate linear system solves and convex optimization, by exploiting low rank structure. Employing randomized low rank approximation, we design a new randomized preconditioner for the conjugate gradient method, and a method called NysADMM, for composite convex optimization. These methods come with strong theoretical and numerical support. Indeed, a simple implementation of NysADMM solves important problems like lasso, logistic regression, and support vector machines 2–42x faster than standard solvers.

## [03373] Sketched Gaussian Model Linear Discriminant Analysis via the Randomized Kaczmarz Method

**Format :** Talk at Waseda University

**Author(s) :** Jocelyn T. Chi (Rice University)Deanna Needell (University of California at Los Angeles)

**Abstract :** We present an iterative randomized approach to Gaussian model linear discriminant analysis (LDA) for large data. Harnessing a least squares formulation, we mobilize the stochastic gradient descent framework and obtain a sketched classifier that is very comparable to full data LDA. Our convergence guarantees for the sketched predictions on new data account for both modeling and algorithmic randomness. Our experiments demonstrate that sketched LDA can offer a very viable alternative for very large data.

## [03665] Moment Estimation of Nonparametric Mixtures Through Implicit Tensor Decomposition

**Format :** Talk at Waseda University

**Author(s) :** Joe Kileel (UT Austin)Yifan Zhang (UT Austin)

**Abstract :** I will present methods to estimate conditionally-independent multivariate mixture models, without assuming parameterizations of the distributions. Following the method of moments, I will tackle an incomplete tensor decomposition problem to compute the mixing weights and componentwise means. Then I will explain how to compute

the cumulative distribution functions and other statistics through linear solves. Crucially for computations in high dimensions, methods in this talk evade steep costs associated with high-order tensors, via efficient tensor-free operations.

## [04802] Are sketch-and-precondition least squares solvers numerically stable?

**Format :** Talk at Waseda University

**Author(s) :** Maike Meier (University of Oxford)Yuji Nakatsukasa (University of Oxford)Alex Townsend ( Cornell University)Marcus Webb (University of Manchester)

**Abstract :** Sketch-and-precondition solvers, such as Blendenpik and LSRN, are popular for solving large least squares (LS) problems of the form  $Ax = b$  with  $A \in \mathbb{R}^{m \times n}$  and  $m \gg n$ . In this talk, we show that the sketch-and-precondition technique is not numerically stable for highly ill-conditioned LS problems. We propose an alternative method, which we call *sketch-and-apply*, based on directly applying the randomized preconditioner and show it is numerically stable under moderate conditions.

00107 (3/3) : 4E @E603 [Chair: Yuji Nakatsukasa]

## [04913] RandBLAS and RandLAPACK - Toward Standard Libraries for RandNLA

**Format :** Talk at Waseda University

**Author(s) :** Riley John Murray (ICSI, LBNL, and UC Berkeley)James Demmel (UC Berkeley)Michael Mahoney (ICSI, LBNL, and UC Berkeley)N. Benjamin Erichson (ICSI and LBNL)Maksim Melnichenko (UT Knoxville)Osman Asif Malik (LBNL)Laura Grigori (INRIA Paris and Sorbonne University)Piotr Luszczek (UT Knoxville)Michał Dereżynski (University of Michigan)Miles Lopes (UC Davis)Tianyu Liang (UC Berkeley)Hengrui Luo (LBNL)Jack Dongarra (UT Knoxville)Burlen Loring (LBNL)Parth Nobel (Stanford University)

**Abstract :** This talk concerns an ongoing effort to bring RandNLA further into mainstream computing. It includes highlights from our recently released monograph (arXiv:2302.11474) as well as discussion of software. The software component focuses on our C++ library for sketching called RandBLAS. We showcase RandBLAS' capabilities by using it to implement a recently developed algorithm for pivoted QR decompositions of tall matrices. Experiments show the proposed algorithm is often faster than Intel MKL's unpivoted QR.

## [04810] Error Estimation in Randomized Algorithms for Rank-Revealing Factorizations

**Format :** Online Talk on Zoom

**Author(s) :** Katherine Joyce Pearce (The Oden Institute at the University of Texas at Austin)Chao Chen (The Oden Institute at the University of Texas at Austin)Yijun Dong (The Oden Institute at the University of Texas at Austin)Per-Gunnar Martinsson (The Oden Institute at the University of Texas at Austin)

**Abstract :** Interpolative decompositions involve “natural bases” of row and column subsets of a given matrix that approximately span its row and column spaces.

For large-scale problems, randomized sketching can serve as an initial step in skeleton selection.

In this talk, we describe an adaptive, parallelizable algorithm applying LU with partial pivoting to randomized sketches to determine a target rank for the approximation.

Our algorithm exhibits improved efficiency over adaptive randomized column-pivoted QR while maintaining comparable accuracy.

## [04484] Krylov-aware stochastic trace estimation

**Format :** Talk at Waseda University

**Author(s) :** Tyler Chen (New York University)Eric Hallman (Google)

**Abstract :** We discuss an algorithm for estimating the trace of a matrix function  $f(\mathbf{A})$  using implicit products with a symmetric matrix  $\mathbf{A}$ . Existing methods for implicit trace estimation of a matrix function tend to treat matrix-vector products with  $f(\mathbf{A})$  as a black-box to be computed by a Krylov subspace method. Like other algorithms for implicit trace estimation, our approach is based on a combination of deflation and stochastic trace estimation. However, we take a closer look at how products with  $f(\mathbf{A})$  are integrated into these approaches which enables several efficiencies not present in previously studied methods. In particular, we describe a Krylov subspace method for computing a low-rank approximation of a matrix function by a computationally efficient projection onto Krylov subspace.

## [04463] How and why to "uncompute" the randomized SVD

**Format :** Talk at Waseda University

**Author(s) :** Ethan Nicholas Epperly (California Institute of Technology)

**Abstract :** The randomized SVD is a low-rank approximation procedure and is a foundational tool in randomized matrix computations. This talk introduces a novel “uncomputing” operation in which the randomized SVD approximation is

part\_1

downdated by deleting different columns from the random test matrix. Two examples of the use of this "uncomputing" primitive are presented: estimating the trace of a matrix accessed only through matrix–vector products and estimating the error of the randomized SVD low-rank approximation.

## [00108] Recent Advances on Kinetic and Related Equations

### **Session Time & Room :**

00108 (1/3) : 1C (Aug.21, 13:20-15:00) @G702

00108 (2/3) : 1D (Aug.21, 15:30-17:10) @G702

00108 (3/3) : 1E (Aug.21, 17:40-19:20) @G702

### **Type :** Proposal of Minisymposium

**Abstract :** Kinetic theory has been expanding its frontier and emerged as promising in various fields of engineering and science. At the same time, it has been a source of unsolved mathematical problems at fundamental levels, which are still actively studied. This mini-symposium aims at bringing in international experts on mathematical analysis, modeling, and computation of kinetic theory and related topics, in order to present the field's state-of-the-art results and foster future academic exchanges and collaborations among researchers from different sub-fields. We propose three sessions which include 12 speakers from different generations of the field and 2 leading experts Tai-Ping Liu and Shih-Hsien Yu as chairpersons who can enhance the communication of the groups.

**Organizer(s) :** Jin-Cheng Jiang, Satoshi Taguchi, Hai-Tao Wang, Seok-Bae Yun

**Classification :** 35Q20, 76P05, 82C40, 82D05

### **Minisymposium Program :**

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00108 (1/3) : 1C @G702 [Chair: Satoshi Taguchi]

## [01451] Boundary singularity of a mono-speed Lorentz model for molecules with the infinite-range potential

### **Format :** Talk at Waseda University

**Author(s) :** Shigeru Takata (Kyoto University)Masanari Hattori (Kyoto University)Hayato Iida (Kyoto University)

**Abstract :** Possibility of the diverging gradient of the macroscopic quantity near the boundary is investigated by a mono-speed Lorentz-gas model, with a special attention to the regularizing effect of the grazing collision for the infinite-range potential on the velocity distribution function (VDF) and its influence on the macroscopic quantity. By careful numerical analyses of the steady one-dimensional boundary-value problem, it is confirmed that the grazing collision suppresses the occurrence of a jump discontinuity of the VDF on the boundary. However, as the price for that regularization, the collision integral becomes no longer finite in the direction of the molecular velocity parallel to the boundary. Consequently, the gradient of the macroscopic quantity diverges, even stronger than the case of the finite-range potential. A conjecture about the diverging rate in approaching the boundary is made as well for a wide range of the infinite-range potentials, accompanied by numerical evidences.

## [01849] On the Existence and Regularity for the Stationary Linearized Boltzmann Equation in a Small Domain

### **Format :** Talk at Waseda University

**Author(s) :** I-Kun Chen (National Taiwan University)Ping-Han Chuang (National Taiwan University)Jhe-Kuan Su (National Taiwan University)Chun-Hsiung Hsia (National Taiwan University)Daisuke Kawagoe (Kyoto University)

**Abstract :** We consider the incoming boundary value problem for the stationary linearized Boltzmann equation in a bounded domain with  $C^2$  boundary of positive Gaussian curvature. We prove the existence of  $H^1$  of solutions under assumptions that the boundary data is good enough and the domain is small enough. A counter example is provided to demonstrate the role of the geometry.

## [05464] Regularity estimates for the non-cutoff soft potential Boltzmann equation with typical rough and slowly decaying data

**Format :** Talk at Waseda University

**Author(s) :** Lingbing He (Tsinghua University)Jie Ji (Peking University)

**Abstract :** or the non-cutoff soft potential Boltzmann equation, if the Boltzmann collision operator is strictly elliptic in the  $v$  variable, it is conjectured that the solution to the equation will become infinitely smooth instantly for both spatial and velocity variables for any positive time, even if the initial data has only polynomial decay in high velocity regimes. This conjecture is significant because it is closely connected to the regularity problem of weak solutions, especially for the smoothing property of so-called regular point''. In this work, we show that the conjecture may not hold for the general weak solution due to the degenerate and non-local properties of the collision operator. We demonstrate this in three steps: (i) constructing so-called typical rough and slowly decaying data"; (ii) proving that such data induces only finite smoothing effect for weak solutions in Sobolev spaces; and (iii) proving that this finite smoothing property induces local properties for any positive time, including that the Leibniz rule does not hold for high derivatives of the collision operator (even in the weak sense) and that there is a discontinuity in the  $x$  variable for the average of weak solutions on certain domains.

## [00646] Vanishing angular singularity limit to the hard-sphere Boltzmann equation

**Format :** Talk at Waseda University

**Author(s) :** Jin Woo Jang (Pohang University of Science and Technology)Bernhard Kepka (University of Bonn)Alessia Nota (Università degli Studi dell'Aquila)Juan J. L. Velázquez (University of Bonn)

**Abstract :** In this talk we consider Boltzmann's collision kernel for inverse power law interactions  $U_s(r) = 1/r^{s-1}$  for  $s > 2$  in dimension  $d = 3$ . We introduce the proof of the limit of the non-cutoff kernel to the hard-sphere kernel and give precise asymptotic formulas of the singular layer near  $\theta \simeq 0$  in the limit  $s \rightarrow \infty$ . Consequently, we show that solutions to the homogeneous Boltzmann equation converge to the respective solutions.

00108 (2/3) : 1D @G702 [Chair: Jin-Cheng Jiang]

## [04112] On BGK-type models with velocity-dependent collision frequency

**Format :** Talk at Waseda University

**Author(s) :** Doheon Kim (Hanyang University)Seok-Bae Yun (Sungkyunkwan University)

**Abstract :** In the original Bhatnagar-Gross-Krook (BGK) model, the collision term in the Boltzmann equation is replaced by a simpler expression, so that the model is easier-to-handle and satisfies the conservation laws and the H-Theorem. This model contains the collision frequency as a parameter independent of the particle velocity. In this talk, I will introduce variants of the BGK model which contain velocity-dependent collision frequency, thereby mimicing the behavior of the Boltzmann equation more closely.

## [02844] Green's function for solving IBVP of evolutionary PDEs

**Format :** Talk at Waseda University

**Author(s) :** Hung-Wen Kuo (National Cheng Kung University)

**Abstract :** We propose a new method to solve the initial-boundary value problem for hyperbolic-dissipative PDEs based on the spirit of LY algorithm. Utilizing the idea of Laplace wave train and the notions of Rayleigh surface wave operators, we are able to obtain the complete representations of the Green's functions for the convection-diffusion equation and the drifted wave equation in a half space with various boundary conditions.

## [00644] H"OLDER REGULARITY OF THE BOLTZMANN EQUATION PAST AN OBSTACLE

**Format :** Talk at Waseda University

**Author(s) :** donghyun lee (POSTECH)chanwoo Kim (University of Wisconsin, madison)

**Abstract :** Regularity and singularity of the Boltzmann equation with various shape of domains is a challenging research theme in the Boltzmann theory. In this talk, we discuss about H"older regularity of the Boltzmann equation outside of convex object under specular reflection boundary condition.

**[03811] Solution to the Boltzmann equation without cutoff in  $(L^1 \cap L^p)_k$** **Format :** Talk at Waseda University**Author(s) :** Shota Sakamoto (Kyushu University)Renjun Duan (Chinese University of Hong Kong)Yoshihiro Ueda (Kobe University)**Abstract :** We consider a Cauchy problem of the Boltzmann equation without angular cutoff near the global Maxwellian on the whole space. In this case, the control of the  $L^1$  norm on the Fourier side is not sufficient for global existence due to low-frequency terms. Therefore, we employ the  $L^p$  norm estimates with respect to the frequency to control such parts. This  $L^1 \cap L^p$  strategy will close a priori estimates when combined with a time-weighted energy method.

00108 (3/3) : 1E @G702 [Chair: Seok-Bae Yun]

**[01835] Mixture estimate in fractional sense****Format :** Talk at Waseda University**Author(s) :** Kung-Chien Wu (National Cheng Kung University)**Abstract :** In this talk, we consider the Boltzmann equation with angular-cutoff for very soft potential case. We prove a regularization mechanism that transfers the microscopic velocity regularity to macroscopic space regularity in the fractional sense. A precise pointwise estimate of the fractional derivative of collision kernel, and a connection between velocity derivative and space derivative in the fractional sense are exploited to overcome the high singularity for very soft potential case.**[03301] Dynamical behaviors in stochastic kinetic flocking models****Format :** Talk at Waseda University**Author(s) :** Xiongtao Zhang (Wuhan University)**Abstract :** We will introduce some recent works on the stochastic flocking models. We are interested in the case when the noise is multiplicative and the flocking interaction vanishes at the far field. We will show rigorous proof of mean-field limit (weak or strong) and the emergence of flocking (conditional or unconditional) under various assumptions.**[04712] Kinetic study of a gas undergoing resonant collisions****Format :** Online Talk on Zoom**Author(s) :** Francesco Salvarani (DVRC & University of Pavia)Laurent Boudin (Sorbonne Université)Thomas Borsoni (Sorbonne Université)Julien Mathiaud (CEA & Université de Bordeaux)Alex Rossi (Friedrich-Alexander-Universität Erlangen-Nürnberg)**Abstract :** We study a kinetic model for a gas undergoing résonant collision. After proving the main properties of the model, we study the compactness of the corresponding linearized Boltzmann operator.**[00110] Computation on Supersingular and Superspecial Curves and its Applications****Session Time & Room :** 5D (Aug.25, 15:30-17:10) @G302**Type :** Proposal of Minisymposium**Abstract :** Supersingular and superspecial algebraic curves have been studied in coding theory and cryptography for the last few decades. The applications are based on explicit constructions and computational aspects of such algebraic curves, which give novel and fascinating mathematical challenges. Interestingly, we have different kinds of problems depending on the genus of curves. The supersingular genus 1 curves, i.e., elliptic curves, are a central ingredient in quantum-resistant isogeny-based cryptography. A series of recent research shows that the security of the cryptosystems is closely related to arithmetic on superspecial curves of higher genera, whose study is the main topic in this minisymposium.**Organizer(s) :** Katsuyuki Takashima**Classification :** 14G50, 14H40, 14H45, 14K02, 14Q05**Minisymposium Program :**

00110 (1/1) : 5D @G302 [Chair: Masaya Yasuda]

## [04024] Decomposed Richelot isogenies of Jacobian varieties of hyperelliptic curves and generalized Howe curves

**Format :** Talk at Waseda University

**Author(s) :** Toshiyuki Katsura (University of Tokyo)Katsuyuki Takashima (Waseda University)

**Abstract :** We advance previous studies on decomposed Richelot isogenies (Katsura-Takashima (ANTS 2020) and Katsura (J. Algebra)) which are useful for analysing superspecial Richelot isogeny graphs in cryptography. We first give a characterization of decomposed Richelot isogenies between Jacobian varieties of hyperelliptic curves of any genus. We then define generalized Howe curves, and present two theorems on their relationships with decomposed Richelot isogenies. We also give new examples including a non-hyperelliptic (resp. hyperelliptic) generalized Howe curve of genus 5 (resp. of genus 4).

## [04668] Some explicit arithmetics on curves of genus three and their applications

**Format :** Online Talk on Zoom

**Author(s) :** Tomoki Moriya (University of Birmingham)Momonari Kudo (Fukuoka Institute of Technology)

**Abstract :** A Richelot isogeny between Jacobian varieties is an isogeny whose kernel is included in the 2-torsion subgroup of the domain. In particular, a Richelot isogeny whose codomain is the product of two or more principally polarized abelian varieties is called a decomposed Richelot isogeny. In this talk, I provide some explicit arithmetics on curves of genus 3, including algorithms to compute the codomain of a decomposed Richelot isogeny. I also provide explicit formulae of defining equations for Howe curves of genus 3 as solutions to computing the domain of a decomposed Richelot isogeny. Finally, I give a construction of an algorithm with complexity  $O\sim(p^3)$  (resp.  $O\sim(p^4)$ ) to enumerate all hyperelliptic (resp. non-hyperelliptic) superspecial Howe curves of genus 3.

## [05345] Construction of superspecial curves of higher genera with extra automorphisms

**Format :** Talk at Waseda University

**Author(s) :** Momonari Kudo (Fukuoka Institute of Technology)

**Abstract :** Superspecial curves are one of the most important objects in algebraic geometry over fields of positive characteristic, with applications to coding theory and cryptography, but explicit constructions and enumerations of such curves of higher genera are known to be quite difficult in general. In this talk, we develop several algorithms to construct superspecial curves of higher genera, restricting ourselves to the case of curves with non-trivial automorphisms, e.g., genus-4 hyperelliptic curves with order-6 automorphisms.

## [04048] Several examples of curves whose superspeciality imply maximality or minimality

**Format :** Talk at Waseda University

**Author(s) :** Ryo Ohashi (University of Tokyo)Shushi Harashita (Yokohama National University)

**Abstract :** A curve over the finite field  $\mathbb{F}_q$  of characteristic  $p > 0$  is called maximal (resp. minimal) if the number of its  $\mathbb{F}_q$ -rational points attains the Hasse-Weil upper (resp. lower) bound. Maximal curves have been investigated for their applications to cryptography and coding theory. It is known that maximal or minimal curves over  $\mathbb{F}_{p^2}$  are all superspecial, while superspecial curves over  $\mathbb{F}_{p^2}$  are not necessary maximal nor minimal. However in this lecture, we will present several examples of curves  $C$  which have the following property: If  $C$  is superspecial, then  $C$  is maximal or minimal over  $\mathbb{F}_{p^2}$ .

## [00114] Computational Biology

**Session Time & Room :**

00114 (1/3) : 3E (Aug.23, 17:40-19:20) @A508

00114 (2/3) : 4C (Aug.24, 13:20-15:00) @A508

00114 (3/3) : 4D (Aug.24, 15:30-17:10) @A508

**Type :** Proposal of Minisymposium

**Abstract :** Besides the traditional (experimental) and theoretical biology, computational biology is the third biology. Its mission is to visualize the activities of living things on the screen to understand their backgrounds theoretically and to predict future status for applications. For this purpose, experimental, data, and simulation sciences are applied, but mathematical formulae are obviously necessary. Computational biology is now widely spreading as a new challenge of industrial and applied mathematics. This minisymposium focuses on recent developments in computational biology.

**Organizer(s) :** Takashi Suzuki

**Classification :** 92-08, 92-10

**Minisymposium Program :**

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00114 (1/3) : 3E @A508 [Chair: Takashi Suzuki]

## [05357] Different mathematical models for membrane electroporation: from equivalent circuit to phase-field models

**Format :** Talk at Waseda University

**Author(s) :** Clair Poignard (INRIA Center of Bordeaux Univ.)

**Abstract :** Electroporation is a complex phenomenon consisting of defects creation in membranes subjected to high short electric pulses. The aim of the talk is to present the mathematical challenges in terms of PDEs and numerical analysis of the phenomenon. A comparison from the 90's biophysical models based on Deryagin theory to very recent phase-field model are performed. For each approach, advantages and disadvantages are discussed, in terms of physical meaning and validation with the experimental data.

## [02031] Modeling and characterizing vaccine-elicited antibody responses

**Format :** Talk at Waseda University

**Author(s) :** Shingo Iwami (Nagoya University)

**Abstract :** Recent studies have provided insights into the effect of vaccine boosters on recall immunity. Given a limited global supply of the vaccinations, identifying vulnerable populations with lower sustained vaccine-elicited antibody titers is important to decide target individuals for the booster. Here we investigated longitudinal data among the cohort of the same individuals of 2,526 people in Fukushima, Japan. Antibody titers following a two-dose SARS-CoV-2 vaccination were repeatedly monitored along with the information on lifestyle habits, comorbidities, adverse reactions, and medication. By employing mathematical modeling and machine learning, we characterized the elicited immune response following a two-dose SARS-CoV-2 vaccination.

## [03370] Mathematical analysis of bone metabolism markers in immobilization mice

**Format :** Talk at Waseda University

**Author(s) :** Marwa Akao (Nagoya University)

**Abstract :** Osteoporosis is a disease that affects more than 200 million people around the world. Although the mechanisms are gradually being revealed, osteoporosis cannot really be cured completely. This study aims to develop the most effective prevention for osteoporosis. We developed mathematical models describing interactions with cells related to bone metabolism and changes in bone mass. And we analyzed the data of bone metabolism markers and compared the difference between immobilization mice and normally fed mice.

## [02284] Predicting clinical outcomes of acute liver failure

**Format :** Online Talk on Zoom

**Author(s) :** Raiki Yoshimura (Division of Natural Science, Graduate School of Science, Nagoya University)

**Abstract :** We used clinical data on acute liver failure to develop an approach for predicting its clinical outcomes. Specifically, we employed a supervised machine learning approach to analyze clinical datasets, including blood test data and medication history, at the admission to the hospital, and predicted final state, i.e., survived or died. In addition, we developed a scoring system to predict individual clinical outcomes. The findings of this study are expected to be utilized in actual clinical practice as a basis for initial response decisions and may also be applied to the detection of other signs of acute diseases.

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00114 (2/3) : 4C @A508 [Chair: Isamu Doku]

## [03648] Mathematical investigation into the mechanism of hair follicle morphogenesis

**Format :** Talk at Waseda University

**Author(s) :** Masaharu Nagayama (Hokkaido University)Makoto Okumura (Konan University)Yasuaki Kobayashi (Hokkaido University)Hironobu Fujiwara ( Institute of Physical and Chemical Research)

**Abstract :** Long-term 3D live imaging of hair follicle morphogenesis during development was shown by Fujiwara et al. During hair follicle morphogenesis, basal cells, basement membrane, and mesenchyme were found to undergo dynamic changes. Fujiwara et al. proposed a telescopic model of hair follicle formation based on these results. In this study, to realize this telescope model, we will construct a mathematical model that reproduces 3D cylindrical compartments and investigate by what mechanism the cylindrical compartments are actively formed.

## [03506] Parameter estimation of the compartmental model of systemic circulation describing the Glucose, Insulin and C peptide dynamics

**Format :** Talk at Waseda University

**Author(s) :** Yueyuan Gao (Hokkaido University)Hiroshi Suito (Tohoku University)Hayato Chiba (Tohoku University)Masaharu Nagayama (Hokkaido University)Hideki Katagiri (Tohoku University)

**Abstract :** In this talk, we explain the construction of the mathematical compartmental model of systemic circulation describing the Glucose, Insulin and C peptide dynamics and we present the application of Markov chain Monte Carlo method to estimate the parameters of the model from clinical data.

## [02898] Effective nonlocal kernels on Reaction-diffusion networks

**Format :** Talk at Waseda University

**Author(s) :** Shin-Ichiro Ei (Hokkaido University)

**Abstract :** A new method to derive an essential integral kernel from any given reaction-diffusion network is proposed. Any network describing metabolites or signals with arbitrary many factors can be reduced to a single or a simpler system of integro-differential equations called “effective equation” in the convolution type.

00114 (3/3) : 4D @A508 [Chair: Takashi Suzuki]

## [04349] Mathematical model of mTORC1 pathway sensing intracellular amino-acids and glucose

**Format :** Talk at Waseda University

**Author(s) :** Takanori Nakamura (Ehime University)Shigeyuki Nada (Osaka University)Takashi Suzuki (Osaka University)Masato Okada (Osaka University)

**Abstract :** mTORC1, a master regulator of metabolism, is activated upon Insulin and Amino-acids (AA) addition, but its regulatory mechanism is not fully understood. We therefore constructed an integrated mathematical model of mTORC1 regulation through the two distinct AA- and Insulin-sensing axes. Using the mathematical simulation with experimental data, we found the selective dephosphorylation during AA deprivation, which ensures full mTORC1 activation only upon the concurrently sensing of nutrient Insulin and AA.

## [05379] Mathematical modeling of cancer immune escape

**Format :** Talk at Waseda University

**Author(s) :** Hiroshi Haeno (Tokyo University of Science)Koichi Saeki (Tokyo University of Science)

**Abstract :** A tumor evolves under the pressure of immune responses. Immune checkpoint inhibitors (ICIs) are expected to reactivate antitumor immunity and inhibit tumor progression. Here, we developed a mathematical model of the tumor evolution under immune responses. As a result, we confirmed that patients who had high mutational load were likely to have a durable benefit. Moreover, we found that the growth rate of tumor cells would be informative to identify responders to ICIs.

## [02179] Computational modelling of cancer invasion using organotypic invasion assay data

**Format :** Talk at Waseda University

**Author(s) :** Mark Chaplain (University of St Andrews)Nikolaos Sfakianakis (University of St Andrews)Linnea Franssen (Roche, Basel)

**Abstract :** We present computational simulation results from a three-dimensional hybrid atomistic-continuum model that describes the invasive growth dynamics of individual cancer cells in tissue. The framework explicitly accounts for phenotypic variation by distinguishing between cancer cells of an epithelial-like and a mesenchymal-like phenotype. It part\_1

also describes mutations between these cell phenotypes. The full model consists of a hybrid system of partial and stochastic differential equations describing the evolution of cancer cells, extracellular matrix and matrix-degrading enzymes.

## [05467] The prognostic value of immune infiltration patterns on the outcome of chemotherapy in breast cancer

**Format :** Online Talk on Zoom

**Author(s) :** Nikolaos Ioannis Kavallaris (Karlstad University)

**Abstract :** In this work, based on a breast cancer biopsy dataset, taken from the ADAPT clinical trial, we shed light on the changes of tumor microenvironment after cytostatic chemotherapy. We combine machine learning workflow to identify cell density patterns identifying responders and non-responders. We also develop a dynamic model that allows us to elucidate the reasons of therapy failure. Finally, using our model we can reason on therapy combinations that could improve the therapeutic outcomes.

## [00118] On mathematical modeling and simulation of droplets

**Session Time & Room :**

00118 (1/3) : 1C (Aug.21, 13:20-15:00) @D402

00118 (2/3) : 1D (Aug.21, 15:30-17:10) @D402

00118 (3/3) : 1E (Aug.21, 17:40-19:20) @D402

**Type :** Proposal of Minisymposium

**Abstract :** The mathematical modeling and simulation of droplets is a basic and fundamental problem in the history of fluid mechanics. Droplets can undergo a variety of interesting nonlinear dynamics such as droplet coalescence/break up, electro-wetting, and traveling waves, etc, due to surface tension effects, substrate geometry and material, as well as external physical forces. This minisymposium will present recent advances in the modeling and simulation of droplets and focus on the mathematical challenges arising from different real-world applications.

**Organizer(s) :** Hangjie Ji, Pejman Sanaei  
**Sponsor :** This session is sponsored by the SIAM Activity Group on Computational Science and Engineering.

**Classification :** 76D45, 35Q35, 76D08, 35G31, 65Mxx

**Minisymposium Program :**

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00118 (1/3) : 1C @D402 [Chair: Pejman Sanaei]

## [03374] Plug formation in models of falling viscous films inside tubes

**Format :** Online Talk on Zoom

**Author(s) :** H. Reed Ogrosky (Virginia Commonwealth University)

**Abstract :** Falling viscous liquid films coating the interior of a tube occur in a variety of applications. If the film is thick enough, it may pinch off and form a plug, occluding the tube. In this talk I will discuss recent work examining the impact of surfactant, slip, viscoelasticity, and viscosity stratification on plug formation in a model for film flow. Implications for understanding occlusion in human airways will be discussed.

## [03547] Dipole-type solutions to the thin-film equation

**Format :** Talk at Waseda University

**Author(s) :** Mark Bowen (Waseda University) Thomas Witelski (Duke University)

**Abstract :** We investigate the dynamics of a thin liquid film spreading in a semi-infinite domain  $x \geq 0$ , so that  $x = 0$  corresponds to an edge over which fluid can drain. In particular, we investigate self-similar solutions of the one-dimensional "thin-film" equation (a fourth order degenerate parabolic equation) on  $x \geq 0$ . We find classes of first- and second-kind similarity solutions and describe how these classes are connected. We also discuss the extension of our results to self-similar solutions featuring sign-changes.

**[02422] Thermally-driven coalescence in thin liquid film flowing down a fiber****Format :** Talk at Waseda University**Author(s) :** Hangjie Ji (North Carolina State University) Claudia Falcon (Wake Forest University) Erfan Sedighi (University of California, Los Angeles) Abolfazl Sadeghpour (University of California, Los Angeles) Y. Sungtaek Ju (University of California, Los Angeles) Andrea L. Bertozzi (University of California, Los Angeles)**Abstract :** This paper presents a study on the dynamics of a thin liquid film flowing down a vertical cylindrical fibre under a streamwise thermal gradient. Previous works on isothermal flows have shown that the inlet flow and fibre geometry are the main factors that determine a transition from the absolute to the convective instability flow regimes. Our experiments demonstrate that an irregular wavy pattern and bead coalescence, which are commonly seen in the convective regime, can also be triggered by applying a thermal gradient along the fibre. We develop a lubrication model that accounts for gravity, temperature-dependent viscosity and surface tension to describe the thermal effects on downstream bead dynamics. Numerical simulations of the model show good agreement between the predicted droplet coalescence dynamics and the experimental data.

00118 (2/3) : 1D @D402 [Chair: Hangjie Ji, Pejman Sanaei]

**[01886] Hybrid Asymptotic-Numerical Methods for Two-Phase Flow With Soluble Surfactant****Format :** Talk at Waseda University**Author(s) :** Michael Booty (New Jersey Institute of Technology)**Abstract :** Surfactant molecules diffuse slowly in bulk flows because of their size, so that the Peclet number of surfactant diffusion is large, and transfer between a stretched drop interface and bulk flow occurs in a thin layer adjacent to the interface that is about one thousandth of the drop radius. Analytical and numerical results of asymptotic, boundary integral, and conformal mapping techniques are presented. This is joint work with Michael Siegel, Ryan Atwater and Samantha Evans.**[01260] A phase field model for a drop suspended in viscous liquids under the influence of electric fields****Format :** Talk at Waseda University**Author(s) :** Shixin Xu (Duke Kunshan University) Yuzhe Qin (Shanxi University) Huangxiong Huang (Beijing Normal University)**Abstract :** In this talk, we consider modeling the deformation of a droplet under an electric field. Firstly, we derive the Poisson-Nernst-Planck-Navier-Stokes phase field model based on the energy variational method, and then we obtain a general phase-field leaky dielectric model taking into account the capacitance according to the electroneutrality. Then a detailed asymptotic analysis confirms that the sharp interface limit of our proposed diffusive-interface model is consistent with the sharp interface model. We take a series of numerical experiments to validate the correctness and effectiveness of our model. The numerical result shows the validity of the asymptotic analysis by comparing the diffuse interface method and existing immersed boundary method results. Finally, we compare the deformations for the interface with and without the capacitance. It shows that the capacitance will weak the formation of droplets.**[05478] Phase-field modeling of colloid-polymer mixtures in microgravity****Format :** Talk at Waseda University**Author(s) :** Anand Oza (New Jersey Institute of Technology)**Abstract :** We present a theoretical model for colloid-polymer mixtures in a microgravity environment. The addition of polymer to a colloidal suspension induces weakly attractive forces between the colloids and leads to a three-phase coexistence region, wherein liquid phase "droplets" coexist with a low-density gas phase and a high-density crystal phase. Colloid-polymer mixtures are thus an archetype for modeling phase transition processes, but the details of the observed colloidal structures remain poorly understood. We construct, analyze and numerically simulate a phase-field model for structure evolution in colloid-polymer mixtures. The model consists of the Cahn-Hilliard equation, which describes phase separation processes in multicomponent mixtures, coupled with the Stokes equation for viscous fluid flow. The results of the model are compared against experiments performed on the International Space Station, using data available on the NASA Physical Sciences Informatics system.

00118 (3/3) : 1E @D402 [Chair: Hangjie Ji]

## [02884] Capillary rebound of droplets impacting onto a liquid bath

**Format :** Talk at Waseda University

**Author(s) :** Radu Cimpeanu (University of Warwick)Luke F.L. Alventosa (Brown University)Daniel M. Harris (Brown University)

**Abstract :** We study millimetric drops impacting onto the free surface of a quiescent bath, a canonical scenario which provides excellent opportunities to co-develop experimental, analytical and computational techniques in a rich multi-scale context. We find that increases in gravitational forces or viscosity lead to a decrease in the coefficient of restitution and an increase in the contact time. The inertio-capillary limit defines an upper bound on the coefficient of restitution, depending only on the Weber number.

## [01510] Motion of Liquid Droplets in Gas Channels

**Format :** Talk at Waseda University

**Author(s) :** Marina Chugunova (Claremont Graduate University )

**Abstract :** Understanding of liquid droplets dynamics in gas channels is critical for improvement of performance and durability of the catalysts made of a dense porous material. We derive a mathematical model to study how different surface properties and operating conditions affect the dynamics of liquid droplets. We present multiple numerical simulations of a single droplet dynamics for different sizes of droplets and different choices of contact angles. We show the influence of an air flow to a thin liquid film and analyze traveling wave type solutions.

Joint work with A. Nadim, Y Ruan, and R Taranets

## [02886] On the immersed boundary method in simulating liquid-gas interfaces

**Format :** Talk at Waseda University

**Author(s) :** Pejman Sanaei (Georgia State University)Michael Y. Li (New York University)Daniel Chin (New York University)Charles Puelz (Baylor College of Medicine)

**Abstract :** In this work, we use the immersed boundary method with four extensions to simulate a moving liquid-gas interface on a solid surface. We first define a moving contact line model and implements a static-dynamic friction condition at the immersed solid boundary. The dynamic contact angle is endogenous instead of prescribed, and the solid boundary can be non-stationary with respect to time. Second, we simulate both a surface tension force and a Young's force with one general equation that does not involve estimating local curvature. In the third extension, we splice liquid-gas interfaces to handle topological changes, such as the coalescence and separation of liquid droplets or gas bubbles. Finally, we re-sample liquid-gas interface markers to ensure a near-uniform distribution without exerting artificial forces. We demonstrate empirical convergence of our methods on non-trivial examples and apply them to several benchmark cases, including a slipping droplet on a wall and a rising bubble.

# [00134] Evolution Equations for Interacting Species: Applications and Analysis

**Session Time & Room :**

00134 (1/3) : 2C (Aug.22, 13:20-15:00) @D407

00134 (2/3) : 2D (Aug.22, 15:30-17:10) @D407

00134 (3/3) : 2E (Aug.22, 17:40-19:20) @D407

**Type :** Proposal of Minisymposium

**Abstract :** This mini-symposium brings together leading experts in the field of systems of PDEs arising in the context of interacting particles. Steric effects and interactions between members of opposite or the same species typically lead to systems of nonlocal and cross-diffusion type. The interplay of degenerate parabolicity and nonlocalities leads to a myriad of interesting emergent behaviours including pattern formation and phase separation. At the same time, these systems pose a variety of challenging analytical mathematical problems including the dramatic loss of regularity at the onset of phase separation. Thus, new analytical techniques and reliable numerical methods are needed.

**Organizer(s) :** Jan-Frederik Pietschmann, Markus Schmidtchen, Havva Yoldaş

**Classification :** 82-XX, 35-XX, Interacting Particle Systems, Evolution Equations, Pattern Formation

**Minisymposium Program :**

## [05128] Evolution Equations for Interacting Species: Applications and Analysis

**Format :** Online Talk on Zoom

**Author(s) :** Jan-Frederik Pietschmann (University of Augsburg) Markus Schmidtchen (Technische Universität Dresden) Havva Yoldaş (Delft University of Technology)

**Abstract :** This talk provides an overview of the mini-symposium's topic of systems of PDEs arising in the context of interacting particles. Steric effects and interactions between members of opposite or the same species typically lead to systems of nonlocal and cross-diffusion type. The interplay of degenerate parabolicity and nonlocalities leads to a myriad of interesting emergent behaviours including pattern formation and phase separation. At the same time, these systems pose a variety of challenging analytical mathematical problems including the dramatic loss of regularity at the onset of phase separation. Thus, new analytical techniques and reliable numerical methods are needed.

## [05084] A Keller-Segel type approximation to a cell population dynamics model

**Format :** Talk at Waseda University

**Author(s) :** Hideki Murakawa (Ryukoku University)

**Abstract :** We deal with a cell population dynamics model with nonlocal advection term. Approximating non-local advection as a local problem can be useful for analysis and numerical analysis of the problem. In this talk, we present a Keller-Segel type approximation to the cell population dynamics model. The approximation consists only of local terms. We discuss convergence of the approximation and introduce some applications. This is a joint work with Yoshitaro Tanaka.

## [04550] Convergence of position-based dynamics for first-order particle systems with volume exclusion

**Format :** Talk at Waseda University

**Author(s) :** Steffen Plunder (Kyoto University, ASHBi) Sara Merino-Aceituno (University of Vienna)

**Abstract :** To simulate first-order particle systems with volume exclusion, we adapted the position based dynamics (PBD) method from computer graphics. PBD is a simple, fast and explicit time-stepping method which is unconditionally stable.

Our contribution is the first convergence proof for PBD for first-order systems. Our proof uses the theory of differential inclusions on uniformly prox-regular sets and a new error estimate for alternating projections.

We successfully applied the method in various applications in developmental biology.

## [04803] Graph-to-local limit for the nonlocal interaction equation

**Format :** Talk at Waseda University

**Author(s) :** Georg Heinze (University of Augsburg)

**Abstract :** In this talk I will discuss a proof of existence of solutions for the nonlocal interaction equation in Euclidean space using a graph-based nonlocal approximation. The graph equations are induced by an upwind interpolation, which leads to non-symmetric graph gradient structures that nevertheless converge to a symmetric Wasserstein-type local gradient structure. Furthermore, the flexibility of our graph model allows us to introduce a tensor to modify the geometry underlying the limiting model.

## [05193] A model for territorial dynamics: from particle to continuum

**Format :** Online Talk on Zoom

**Author(s) :** Alethea Barbaro (TU Delft) Abdulaziz Alsenafi (Kuwait University)

**Abstract :** Many species, including our own, demonstrate territoriality, with individuals or groups marking their territories either chemically or visually. Here, we present an agent-based lattice model for territorial development. In this model, there are several groups; agents from each group put down that group's territorial markings as they move on the lattice. Agents move away from areas with territorial markings which do not belong to their own group. The model was motivated by gangs expressing territoriality through graffiti markings, though the model itself could be applicable in any chemo-repellent situation. We show that this model undergoes a phase transition between well-mixed dynamics and the formation of distinct territories as parameters are varied. We formally derive a system of coupled convection-

diffusion equations from this model. The system is cross-diffusive due to the avoidance of other groups' markings. Using the PDE system, we pinpoint the critical value for the phase transition.

## [04662] A variational approach for an existence result for a cross-diffusion model

**Format :** Talk at Waseda University

**Author(s) :** Havva Yoldaş (Delft University of Technology)Filippo Santambrogio (Université Claude Bernard - Lyon 1)Romain Ducasse (Université Paris Cité)

**Abstract :** In this talk, we look at a cross-diffusion system consisting of two Fokker-Planck equations where the gradient of the density for each species acts as a potential for the other one. The system is the gradient flow for the Wasserstein distance of a functional which is not lower semi-continuous, and the system is not well-posed. We compute the convexification of the integral and provide an existence proof in a suitable sense for the gradient flow of the corresponding relaxed functional.

## [04745] A degenerate cross-diffusion system as the inviscid limit of a nonlocal tissue growth model

**Format :** Talk at Waseda University

**Author(s) :** Tomasz Dębiec (University of Warsaw)

**Abstract :** In recent years, there has been a spike in interest in multi-phase tissue growth models. Depending on the type of tissue, the velocity is linked to the pressure through Stoke's law, Brinkman's law or Darcy's law. While each of these velocity-pressure relations has been studied in the literature, little emphasis has been placed on the fine relationship between them. In this talk, we want to address this dearth of results in the literature, providing a rigorous argument that bridges the gap between a viscoelastic tumour model (of Brinkman type) and an inviscid tumour model (of Darcy type).

## [04637] Proposing a Finite Volume Method for a Kinetic Model for Interacting Species

**Format :** Talk at Waseda University

**Author(s) :** Julia Ines Mareike Hauser (TU Dresden)

**Abstract :** We consider a system of two kinetic equations coupled by non-local interaction terms which are used to describe systems of indistinguishable agents such as flocks of birds.

In this talk we propose an upwind finite volume method for this model. The method is constructed in such that mass is preserved and positivity is maintained. We show the convergence of the method and we provide explicit error estimates. Finally, we underline our theoretical results with simulations.

00134 (3/3) : 2E @D407 [Chair: Havva Yoldaş]

## [05038] Mean-field convergence in $L^2$ -norm for a diffusion model with aggregation

**Format :** Online Talk on Zoom

**Author(s) :** Alexandra Holzinger (TU Wien )

**Abstract :** Aggregation effects appear in many applications arising from biology and physics which makes it interesting to study this phenomena also in mean-field settings. It is well-known that a class of local diffusion-aggregation equations can be derived by using classical mean-field limits. In this talk I will explain the benefits we get by showing a result in  $L^2$ -norm and how this is connected to fluctuations around the mean-field limit.

## [04613] Macroscopic limits of kinetic equations for the switch in cell migration via binary interactions

**Format :** Talk at Waseda University

**Author(s) :** Gissell Estrada-Rodriguez (University of OxfordU)

**Abstract :** Motivated by experimental results on the immune response to cancer, we considered a system of particles, I, in an

inactive state, where they follow a nonlocal (Levy) movement. After a collision with particles in population D, they change to an active state, A, resulting in a more localised (Brownian) movement. Activation is described via binary interactions between I and D. Moreover, cell motion is represented as a velocity-jump process, with the running time of I following a long-tailed distribution, which is consistent with a Levy walk, and the running time of A following a Poisson distribution, which corresponds to Brownian motion. We formally show that the macroscopic limit of the model comprises a coupled system of balance equations for the one-particle distribution functions of populations I, D and A. The modelling approach presented here and its possible generalisations are expected to find applications in the study of part\_1

the immune response to cancer and in other biological contexts in which switch from non-local to localised migration patterns occurs.

### [04647] Towards a new mathematical model of the visual cycle

**Format :** Talk at Waseda University

**Author(s) :** Luca Cesare Biagio Alasio (Sorbonne UniversitéSorbonne Université)

**Abstract :** The visual cycle is a fundamental bio-chemical process allowing photoreceptors to convert light into electrical signals and return to the dark state. I will present a new mathematical model involving coupled ODEs and PDEs for the kinetics of retinal photo-sensitive molecules after light exposure. This reaction-diffusion-type model provides a first step in the study of the accumulation of toxic by-products in the eye in connection with retinal diseases such as age-related macular degeneration.

### [04418] Structured Model for the Size-spectrum Evolution in Aquatic Ecosystems

**Format :** Talk at Waseda University

**Author(s) :** Laura Kanzler (CEREMADE - Université Paris-Dauphine)

**Abstract :** Trophic interactions between animals in the ocean were matter of interest since the 60', where it was quickly discovered that the individuals' body size acts as 'master trait' in food webs of animals, giving rise to emergent distributions of biomass, abundance and production of organisms.

We propose and investigate a deterministic jump-growth model of Boltzmann type, aiming to capture this emergence phenomenon in aquatic ecosystems. The equation of interest is derived from individual based dynamics governed by a stochastic process. Following the observation of the body mass being the crucial trait in these dynamics it is based on the assumption that binary interactions between individuals in the ecosystem take place: A predator feeding on a prey, which then results in growth of the predator with assimilating a certain (usually very small) amount of its prey's mass as well as plankton production. Analytical results in various parameter regimes are discussed and numerical simulations underlying these observations are given.

## [00135] Nonlinear PDEs and related diffusion phenomena

**Session Time & Room :**

00135 (1/3) : 4E (Aug.24, 17:40-19:20) @G602

00135 (2/3) : 5B (Aug.25, 10:40-12:20) @G602

00135 (3/3) : 5C (Aug.25, 13:20-15:00) @G602

**Type :** Proposal of Minisymposium

**Abstract :** Diffusion equations have a primary role in the description and modeling of several physical phenomena. A classical prototype is the heat equation, deriving from Fourier's law, which is by now a widely studied topic within the mathematical community, both in Euclidean and non-Euclidean frameworks such as manifolds or metric-measure spaces. In the last decades, many nonlinear and nonlocal versions of this equation and related ones have been proposed and analyzed, which gave rise to challenging mathematical problems. We aim at gathering international experts and talented young researchers that will discuss the most recent advances on the subject.

**Organizer(s) :** Kazuhiro Ishige, Tatsuki Kawakami, Matteo Muratori

**Classification :** 35Kxx, 35Rxx, 39Bxx, 58Jxx, 60Hxx

**Minisymposium Program :**

00135 (1/3) : 4E @G602 [Chair: Kazuhiro Ishige]

### [03392] Boundary Regularity of Local and Nonlocal Equations

**Format :** Talk at Waseda University

**Author(s) :** Ki-Ahm Lee (Seoul National University)

**Abstract :** In this talk, we are going to discuss boundary regularities of various degenerate local equations and nonlocal equations.

Diffusion rates deform undefined geometry related to diffusion and the corresponding distance function

makes an important role in the theory of regularity.  
And then we will also discuss the possible applications.

## [04308] Well-posedness with large data for a weighted porous medium equation

**Format :** Talk at Waseda University

**Author(s) :** Troy Pettitt (Politecnico di Milano)Matteo Muratori (Politecnico di Milano (Italy))

**Abstract :** The large data problem for the porous medium equation is to determine the largest class of initial data for which local well-posedness is guaranteed for the Cauchy problem. We review the classical results by Widder for the heat equation  $u_t = \Delta u$ . The corresponding problem for the porous medium equation  $u_t = \Delta u^m$  for  $m > 1$  was solved in the 1980s. We extend these results for weighted equations  $\rho(x)u_t = \Delta u^m$  for  $\rho(x) \cong |x|^{-\gamma}$  for  $\gamma \in (0, 2)$ .

## [04047] Results on the Stokes eigenvalue problem under Navier boundary conditions

**Format :** Talk at Waseda University

**Author(s) :** Alessio Falocchi (Politecnico di Milano)Filippo Gazzola (Politecnico di Milano)

**Abstract :** We study the Stokes eigenvalue problem under Navier boundary conditions in 2D or 3D bounded domains with connected boundary of class  $C^1$ . Differently from the Dirichlet boundary conditions, zero may be the least eigenvalue. We fully characterize the domains where this happens. We then consider the general version of the problem in any space dimension with  $n \geq 2$ , characterizing the kernel of the strain tensor for solenoidal vector fields with homogeneous normal trace.

## [03585] Weighted Trudinger-Moser inequalities in the subcritical Sobolev spaces

**Format :** Talk at Waseda University

**Author(s) :** Megumi Sano (Hiroshima University)

**Abstract :** Inspired by Ni's result about the H' enon equation with nonlinear term which has the strong polynomial growth beyond the Sobolev critical growth, we consider the exponential growth beyond the polynomial growth in a maximization problem. Also we discuss the optimality and the attainability of our maximization problem. Our inequalities are regarded as subcritical versions of the Trudinger-Moser inequalities in the critical Sobolev spaces. This is a joint work with Masahiro Ikeda(RIKEN/Keio Univ.) and Koichi Taniguchi(Tohoku Univ.).

00135 (2/3) : 5B @G602 [Chair: Matteo Muratori]

## [03273] First order fully nonlinear nonlocal evolution equations

**Format :** Talk at Waseda University

**Author(s) :** Takashi Kagaya (Muroran Institute of Technology)Qing Liu (Okinawa Institute of Science and Technology)Hiroyoshi Mitake (University of Tokyo)

**Abstract :** This talk is concerned with geometric motion of a closed surface whose normal velocity depends on a nonlocal quantity of the enclosed region. Using the level set formulation, we study a class of first order nonlocal evolution equations in the framework of viscosity solution theory. We prove the uniqueness of solutions by establishing a comparison principle. Our existence result is based on careful analysis on parallel surfaces and an optimal control interpretation. We also mention several properties of the solution such as quasiconvexity preserving, fattening phenomenon and large time behavior.

## [02461] The generalized porous medium equation on graphs: Existence and uniqueness of solutions with $l^1$ data

**Format :** Talk at Waseda University

**Author(s) :** Davide Bianchi (Harbin Institute of Technology (Shenzhen))

**Abstract :** We study solutions of the generalized porous medium equation on infinite graphs. For nonnegative or nonpositive integrable data, we prove the existence and uniqueness of mild solutions on any graph. For changing sign integrable data, we show existence and uniqueness under extra assumptions such as local finiteness or a uniform lower bound on the node measure.

## [03236] Global regularity estimates for the Poisson equation on complete manifolds

**Format :** Talk at Waseda University

**Author(s) :** Ludovico Marini (University of Milano-Bicocca (soon at Fukuoka University))Stefano Meda (University of Milano-Bicocca)Stefano Pigola (University of Milano-Bicocca)Giona Veronelli (University of Milano-Bicocca)

**Abstract :** In this talk, we investigate the validity of first and second-order, global  $L^p$  estimates for the solutions of the Poisson equation.

While these estimates always hold on  $\mathbb{R}^n$ , on complete non-compact manifolds their validity is strongly influenced by the large-scale geometry.

I will present some positive results and discuss the sharpness of certain assumptions through counterexamples.

This is a joint work with Stefano Meda, Stefano Pigola and Giona Veronelli of the University of Milano-Bicocca.

## [03203] Radial solutions to a semilinear equation on Riemannian models

**Format :** Talk at Waseda University

**Author(s) :** Elvise Berchio (Politecnico di Torino)Alberto Ferrero (Università del Piemonte Orientale)Debdip Ganguly (Indian Institute of Technology Delhi)Prasun Roychowdhury (National Center for Theoretical Sciences)

**Abstract :** We provide a classification with respect to asymptotic behaviour, stability and intersections properties of radial smooth solutions to the equation  $\Delta_g u = e^u$  on Riemannian models. Our assumptions include Riemannian manifolds with sectional curvatures bounded or unbounded from below. As it is well-known in the Euclidean case, intersection and stability properties are influenced by the dimension; here the analysis highlights properties of solutions that cannot be observed in the flat case.

00135 (3/3) : 5C @G602 [Chair: Tatsuki Kawakami]

## [03548] Quasi self-similarity and its application to the global in time solvability of a superlinear heat equation

**Format :** Talk at Waseda University

**Author(s) :** Yohei Fujishima (Shizuoka University)

**Abstract :** We discuss the global in time existence of solutions for a superlinear heat equation. In particular, we determine the critical decay rate of initial functions for the global existence of solutions by introducing a quasi self-similar solution for the problem.

## [03604] Stochastically perturbed log diffusion equations

**Format :** Talk at Waseda University

**Author(s) :** Reika Fukuizumi (Waseda University)

**Abstract :** We will present a result on the existence and uniqueness of the solution for the stochastic fast logarithmic equation with a Stratonovich multiplicative noise in  $\mathbb{R}^d$  for  $d \geq 3$ . We overcome several technical difficulties due to the degeneracy properties of the logarithm and to the fact that the problem is treated in an unbounded domain. This is a joint work with Ioana Ciotir (INSA Rouen, France) and Dan Goreac (Univ Paris Est, France and Shandong University, China).

## [03225] Spreading and extinction of solutions to the logarithmic diffusion with a logistic reaction

**Format :** Talk at Waseda University

**Author(s) :** Masahiko Shimojo (Tokyo Metropolitan University)Eiji Yanagida (University of Tokyo)Harunori Monobe (Osaka Metropolitan University)

**Abstract :** Logarithmic diffusion is observed in several fields of science, such as the central limit approximation of Carleman's model based on the Boltzmann equation, a model for long Van-der-Waals interactions in thin fluid films, and the evolution of conformal metric under the Ricci flow on the plane. We focus on the spreading and extinction phenomena of the solution to the logarithmic diffusion equation on a line, in the presence of a logistic reaction term. A Liouville-type theorem will be introduced to understand the extinction and interfacial phenomena from the point of entire solutions.

## [03474] Characterization of F-concavity preserved by the Dirichlet heat flow

**Format :** Talk at Waseda University

**Author(s) :** Asuka Takatsu (Tokyo Metropolitan University) Paolo Salani (University of Florence) Kazuhiro Ishige (The University of Tokyo)

**Abstract :** F-concavity is a generalization of power concavity and, actually, the largest available generalization of the notion of concavity. We characterize the F-concavities preserved by the Dirichlet heat flow in convex domains on Euclidean space, and complete the study of preservation of concavity properties by the Dirichlet heat flow, started by Brascamp and Lieb in 1976 and developed in some recent papers.

## [00137] Mathematical Aspects of Multiscale Phenomena in Materials and Complex Fluids

**Session Time & Room :**

00137 (1/3) : 3C (Aug.23, 13:20-15:00) @E802

00137 (2/3) : 3D (Aug.23, 15:30-17:10) @E802

00137 (3/3) : 3E (Aug.23, 17:40-19:20) @E802

**Type :** Proposal of Minisymposium

**Abstract :** The mini-symposium will focus on mathematical aspects of multiscale phenomena in materials and complex fluids. New scientific problems along with novel mathematical techniques and computational tools have emerged from the study of multiscale phenomena, for example, in polycrystalline materials, biomaterials, flow through porous media, as well as liquid crystals, to name a few. The mini-symposium will bring together experts in the area of mathematical aspects of materials and complex fluids and will feature talks on the latest advances in the field that range from mathematical modeling and analysis of partial differential equations to algorithm design, simulation and data analysis.

**Organizer(s) :** Yekaterina Epshteyn, Chun Liu, Masashi Mizuno

**Classification :** 74Hxx, 76Txx, 35Qxx, 65Mxx, Materials, Complex Fluids, Modeling, Analysis of PDEs, Simulation

**Minisymposium Program :**

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00137 (1/3) : 3C @E802 [Chair: Chun Liu]

## [00142] New perspectives on modeling and analysis of grain growth in polycrystals

**Format :** Talk at Waseda University

**Author(s) :** Yekaterina Epshteyn (University of Utah) Katayun Barmak (Columbia University) Chun Liu (IIT) Masashi Mizuno (Nihon University)

**Abstract :** Grain growth in polycrystals is a very complex multiscale process. It can be regarded as the anisotropic evolution of a large cellular network, and can be described by a set of deterministic local evolution laws for the growth of an individual grain combined with stochastic models for the interaction between them. In this talk, we will present new perspectives on modeling, simulation and analysis of the evolution of the grain boundary network in polycrystalline materials.

## [00183] Entropy dissipation methods for Nonlinear inhomogeneous Fokker-Planck models

**Format :** Talk at Waseda University

**Author(s) :** Masashi Mizuno (Nihon University) Yekaterina Epshteyn (University of Utah) Chun Liu (Illinois Institute of Technology) Chang Liu (University of Utah)

**Abstract :** This talk presents long-time asymptotic behavior for the nonlinear Fokker-Planck model: First, for the linear Fokker-Planck equation, we reformulate the entropy dissipation methods with the help of the velocity vector in the continuity equation. Next, we derive the evolution equation for the velocity vector for the nonlinear Fokker-Planck model. Finally, we give a sufficient condition to extend the entropy dissipation method to the nonlinear Fokker-Planck model.

## [00198] Structure-preserving variational discretizations to generalized gradient flows

**Format :** Online Talk on Zoom

**Author(s) :** Chun Liu (Illinois Institute of Technology)Yiwei Wang (University of California, Riverside)

**Abstract :** We'll present a numerical framework for developing structure-preserving variational schemes for various complex fluids models built by the energetic variational approach. The numerical approach starts with the energy-dissipation law of the underlying system and can combine different spatial discretizations, including Eulerian, Lagrangian, particle, and neural-network-based methods. The numerical procedure guarantees the developed schemes are energy stable and can preserve the intrinsic physical constraints. Several applications of this numerical approach will be discussed.

## [00248] Towards upscaling and simulation of coupled [THM] systems with applications to permafrost modeling

**Format :** Online Talk on Zoom

**Author(s) :** Małgorzata Peszynska (Oregon State University)Oregon State UniversityNaren Vohra (Oregon State University)

**Abstract :** In the talk we discuss our progress towards multiscale computational modeling of coupled processes in permafrost, frozen ground which is ubiquitous in the Arctic. We focus on its active layer close to the surface whose depth is changing due to changing climate conditions, and we model its thermal state (temperature, and phase status: frozen or thawed), hydrological conditions, and mechanical response to hydrological and thermal controls. We present convergence studies and upscaling from porescale.

00137 (2/3) : 3D @E802 [Chair: Yekaterina Epshteyn]

## [00202] Diffuse-interface approach to competition between viscous flow and diffusion in pinch-off dynamics

**Format :** Talk at Waseda University

**Author(s) :** Weizhu Bao (National University of Singapore)Fukeng Huang (National University of Singapore)Tiezheng Qian (Hong Kong University of Science and Technology)

**Abstract :** In this talk, we present numerical simulations for the pinch-off dynamics in the Stokes regime and the diffusion-dominated regime by adopting the Cahn-Hilliard-Navier-Stokes model derived by applying Onsager's variational principle. The Cahn-Hilliard-Navier-Stokes model is solved by using an accurate and efficient spectral method in a cylindrical domain with axisymmetry. Ample numerical examples are presented to show the pinch-off processes in the Stokes regime and the diffusion-dominated regime, respectively. In particular, the crossover between these two regimes is investigated numerically and analytically to reveal how the scaling behaviors of similarity solutions are to be qualitatively changed as the characteristic length scale is inevitably accessed by the pinching neck of the interface. Discussions are also provided for numerical examples that are performed for the breakup of long liquid filaments and show qualitatively different phenomena in different scaling regimes. This is a joint work with Fukeng Huang and Tiezheng Qian.

## [00195] Multiscale analysis of nonlinear material models with carrier kinetics

**Format :** Talk at Waseda University

**Author(s) :** Qing Xia (KTH Royal Institute of Technology)Ludmila Prokopeva (Purdue University)William Henshaw (RPI)Alexander Kildishev (Purdue University)Gregor Kovacic (RPI)Jeffrey Banks (RPI)Donald Schwendeman (RPI)

**Abstract :** In this talk, we introduce Maxwell-Bloch equations for modeling interactions between light and nonlinear optics. The model is based on real-valued rate equations, which describe kinetics of electrons between the ground state and excited states in the multi-level atomic system. We will show the rate equation approach is connected to the complex-valued density matrix approach via the Schrödinger's equation. Different multi-level atomic systems will be shown and multi-scale analysis is performed.

## [00209] Energetic-variational particle-based method for Fokker-Planck Models.

**Format :** Talk at Waseda University

**Author(s) :** Kaitlin O'Dell (University of Utah)Yekaterina Epshteyn (University of Utah)Chun Liu (Illinois Institute of Technology)

**Abstract :** Fokker-Planck models with energy-dissipation structures arise in many scientific and engineering applications. We present a novel energetic-variational particle-based approach for simulation of such nonlinear high-

part\_1

dimensional Fokker-Planck systems which cannot be solved using traditional numerical methods. First, we compare the performance of the proposed particle-based scheme with the finite-volume structure-preserving method on low-dimensional Fokker-Planck systems. Then, we apply new method for the analysis of the high-dimensional Fokker-Planck equations that describe grain boundaries dynamics in polycrystalline materials.

## [00214] Phase transitions in near-liquid solids

**Format :** Talk at Waseda University

**Author(s) :** Yury Grabovsky (Temple University)Lev Truskinovsky (ESPCI)

**Abstract :** We consider a class of two-dimensional compressible Hadamard materials with very small shear modulus and a double-well potential for the energy as a function of specific volume. Such energy is not rank one convex and is in need of relaxation. While computing energy relaxation seems hopeless, identifying its binodal - the boundary separating stable and unstable homogeneously deformed configurations seems more tractable. I will describe several necessary and sufficient conditions for stability and show how they allow us to bound hydrostatic strains on the binodal. Then, in a surprising twist, I will show how the optimality of our bound would generate an excellent approximation to the entire binodal. This is a joint work with Lev Truskinovsky.

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00137 (3/3) : 3E @E802 [Chair: Masashi Mizuno]

## [00243] A finer singular limit of the Kobayashi-Warren-Carter type functional and its gradient flow

**Format :** Talk at Waseda University

**Author(s) :** Masaaki Uesaka (Arithmer, Inc.)Yoshikazu Giga (the University of Tokyo)Koya Sakakibara (Okayama University of Science)Jun Okamoto (Kyoto University)

**Abstract :** We consider the singular limit of the Kobayashi-Warren-Carter type energy, which is derived from the physical model of grain boundary motion in polycrystals. The KWC-type energy contains the weighted total variation, and hence we must employ a topology finer than  $L^1$  to capture the singular limit's behavior in detail. We shall explain the key result of the singular limit of KWC-type energy and the behavior of its gradient flow.

## [00249] Variational modeling of fluid in poroelastic medium

**Format :** Talk at Waseda University

**Author(s) :** Arkadz Kirshtein (Tufts University)James Haley Adler (Tufts University)Xiaozhe Hu (Tufts University)

**Abstract :** In this talk I will discuss modeling fluid flow through a deformable porous medium. I will start from introducing a variational approach for fluids and elasticity in Lagrangian coordinates. Next I will discuss an existing approach based on Biot's consolidation model. Ultimately I will introduce a system derived using energetic variational approach and discuss numerical methods and simulations based on it.

## [00226] Phase field model for volume-preserving mean curvature flow

**Format :** Talk at Waseda University

**Author(s) :** Keisuke Takasao (Kyoto University)

**Abstract :** In this talk, we show a global existence of the weak solution for the volume-preserving mean curvature flow. To construct the weak solution, we use the Allen-Cahn equation with non-local term given by the penalty method. We prove the  $L^2$ -estimate of the non-local term and the monotonicity formula for the equation, which are the keys of the proof of the existence theorem.

## [00257] A unified continuum model for grain boundary dynamics incorporating microscopic structure

**Format :** Talk at Waseda University

**Author(s) :** Yang Xiang (Hong Kong University of Science and Technology)

**Abstract :** We develop a unified continuum framework to account for the underlying line defect mechanisms. Conditions on the continuum level are imposed to account for the underlying microscopic mechanisms, which makes the continuum model more efficient to describe the collective behaviors of grain boundary networks at larger length scales.

# [00140] Interacting particle systems: modeling, learning and applications

## Session Time & Room :

00140 (1/2) : 3C (Aug.23, 13:20-15:00) @D407

00140 (2/2) : 3D (Aug.23, 15:30-17:10) @D407

**Type :** Proposal of Minisymposium

**Abstract :** Systems of interacting particles or agents are ubiquitous in science and technology, with new theory and applications developing at a rapid pace. This mini-symposium aims at a cross-fertilization of areas in the study of topics in interacting particle systems, including, but not limited to: their analysis, computational techniques, parametric and nonparametric inference problems, control, interacting particles on graphs, use of interacting particle-based methods in optimization and neural networks, modeling and applications.

**Organizer(s) :** Fei Lu, Mauro Maggioni

**Classification :** 82C22, 49Q99, 35R30, 68T09, 35Q83

## Minisymposium Program :

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00140 (1/2) : 3C @D407 [Chair: Mauro Maggioni]

## [03778] The mean-field limit of non-exchangeable integrate and fire systems

**Format :** Online Talk on Zoom

**Author(s) :** Pierre-Emmanuel Jabin (Pennsylvania State University)Datong Zhou (Pennsylvania State University)

**Abstract :** We investigate the mean-field limit of large networks of interacting biological neurons. The neurons are represented by the so-called integrate and fire models that follow the membrane potential of each neurons and captures individual spikes. However we do not assume any structure on the graph of interactions but consider instead any connection weights between neurons that obey a generic mean-field scaling. We are able to extend the concept of extended graphons, introduced in Jabin-Poyato-Soler, by introducing a novel notion of discrete observables in the system.

## [03624] Weak Form Equation Learning for Interacting Particle System Models of Collective Motion

**Format :** Online Talk on Zoom

**Author(s) :** David Bortz (University of Colorado - Boulder)Daniel Messenger (University of Colorado - Boulder)

**Abstract :** The Weak form Sparse Identification of Nonlinear Dynamics (WSINDY) methodology efficiently identifies governing equations from noisy data. We develop WSINDY for inference of 1st and 2nd-order IPS models as well as a joint model selection and classification method to both learn governing IPS equations and sort individuals into distinct interaction rule classes. We demonstrate the efficiency and proficiency of these methods on several test scenarios, motivated by common cell migration experiments.

## [03774] Mean-field nonparametric estimation of interacting particle systems

**Format :** Online Talk on Zoom

**Author(s) :** Xiaohui Chen (University of Southern California)Rentian Yao (University of Illinois at Urbana-Champaign)Yun Yang (University of Illinois at Urbana-Champaign)

**Abstract :** This talk concerns the nonparametric estimation problem of the distribution-state dependent drift vector field in an interacting  $N$ -particle system. Observing single-trajectory data for each particle, we derive the mean-field rate of convergence for the maximum likelihood estimator (MLE), which depends on both Gaussian complexity and Rademacher complexity of the function class. In particular, when the function class contains  $\alpha$ -smooth Hölder functions, our rate of convergence is minimax optimal on the order of  $N^{-\frac{\alpha}{d+2\alpha}}$ . Combining with a Fourier analytical deconvolution estimator, we derive the consistency of MLE for the external force and interaction kernel in the McKean-Vlasov equation.

## [04754] Game-based learning of interaction rules for rational agents

**Format :** Online Talk on Zoom

**Author(s) :** Mauro Bonafini (University of Verona)Massimo Fornasier (Technical University of Munich)Bernhard Schmitzer (University of Göttingen)

**Abstract :** We introduce novel multi-agent interaction models obtained as fast-reaction limits of evolutionary games. We

discuss the well-posedness of these models and the learnability of individual payoff functions from observation data. We formulate the payoff learning as a variational problem, minimizing the discrepancy between the observations and the predictions by the payoff function. The abstract framework is fully constructive and numerically implementable. We illustrate this on computational examples.

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00140 (2/2) : 3D @D407 [Chair: Fei Lu]

## **[04464] Data-driven discovery of interacting particle systems with Gaussian Processes**

**Format :** Talk at Waseda University

**Author(s) :** Sui Tang (University of California Santa Barbara) Charles Kulick (University of California Santa Barbara) Jinchao Feng (Johns Hopkins University)

**Abstract :** We present a data-driven approach for discovering interacting particle models with latent interactions. Our approach uses Gaussian processes to model latent interactions, providing an uncertainty-aware approach to modeling interacting particle systems. We demonstrate the effectiveness of our approach through numerical experiments on prototype systems and real data. Moreover, we develop an operator-theoretic framework to provide theoretical guarantees for the proposed approach. We analyze recoverability conditions and establish the statistical optimality of our approach.

## **[03149] The mean field limit of random batch interacting particle systems**

**Format :** Talk at Waseda University

**Author(s) :** Lei Li (Shanghai Jiao Tong University)

**Abstract :** The Random Batch Method proposed in our previous work (J Comput Phys, 2020) is not only a numerical method for interacting particle systems and its mean-field limit, but also can be viewed as a new model in which particles interact, at discrete time, with randomly selected mini-batch of particles. We investigate the mean-field limit of this model as the number of particles tends to infinity. The mean field limit now exhibits some new features. We will not only justify this mean-field limit (discrete in time) but will also show that the limit approaches to the solution of a nonlinear Fokker-Planck equation as the discrete time step goes to zero.

## **[04827] Neural parameter calibration for large-scale multi-agent systems**

**Format :** Talk at Waseda University

**Author(s) :** Thomas Gaskin (University of Cambridge)

**Abstract :** I present a method to calibrate multi-agent systems to datasets using neural networks, allowing for uncertainty quantification in a manner that reflects both the noise on the data as well as the non-convexity of the parameter estimation problem. I will discuss applications to various different examples, including learning entire network adjacency matrices, and give a comparative analysis of the method's performance in terms of speed, prediction accuracy, and uncertainty quantification to classical techniques.

## **[05244] Non-local regularization of Semilinear PDE for Probability Density Stabilization**

**Format :** Talk at Waseda University

**Author(s) :** Karthik Elamvazhuthi (University of California, Riverside)

**Abstract :** In this talk, I will present some recent work on a particle method for numerically simulating a class of semilinear PDEs that provide strategies for probability density stabilization. These have important applications in problems such as sampling and multi-agent control. We will consider a semilinear diffusion model in which the reaction parameters are to be designed so that the solution of PDE converges to a target probability density. Since the parameters of these PDEs depend on the local density, they are not suitable for implementation on a finite number of particles. We construct a particle method by regularizing the local dependence to construct a non-local PDE. While the nonlocal approximations make numerical implementation easier, their local limits have good analytical properties from the point of view of understanding long-term behavior. Motivated by applications in robotics, the method also easily generalizes to situations where the particle diffusions are degenerate and hence, not elliptic, but only hypoelliptic.

## [00143] Recent advances in stochastic optimal control and contract theory

**Session Time & Room :** 5D (Aug.25, 15:30-17:10) @D501

**Type :** Proposal of Minisymposium

**Abstract :** The aim of this session is to bring together some of the most active junior researchers in the areas of stochastic optimal control, with an emphasis on applications to contract theory and principal-agent problems. It will be a perfect and timely opportunity to take stock of the recent progresses in these very trendy topics, as well as to highlight the deep links that they share. In particular, a specific attention will be put on relationships with mean-field and Stackelberg games, McKean-Vlasov optimal control, and time-inconsistent optimal control problems.

**Organizer(s) :** Dylan Possamai  
**Sponsor :** This session is sponsored by the SIAM Activity Group on Financial Mathematics and Engineering.

**Classification :** 91B41, 60H99, 93E20

**Minisymposium Program :**

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00143 (1/1) : 5D @D501

### [00182] Mean field optimal stopping and applications in contract theory

**Author(s) :** Mehdi Christian Talbi (ETH Zurich)Thibaut Mastrolia (UC Berkeley)

**Abstract :** Mean field optimal stopping problems correspond to optimization problems where a central planner controls a distribution of interacting agents by assigning each of them a stopping time. After explaining how these problems can be studied through dynamic programming, we propose an application to contract theory: one Principal proposes contracts to interacting Agents, and each contract includes a continuous payment and a retirement time, which leads the Principal to solve a mixed control-and-stopping mean field problem.

### [00242] A stochastic target approach to Stackelberg games and moral hazard with constraints

**Author(s) :** Emma Hubert (Princeton University)

**Abstract :** In this talk, we provide a unifying framework for Stackelberg games and principal-agent problems with moral hazard and constraints on the terminal payment. The main idea is that this type of problems can be reformulated as more standard control problems with stochastic target. Indeed, the agent's problem can be rewritten as a BSDE, controlled by the principal, and then the constraint on the terminal payment is equivalent to a terminal constraint on this controlled process.

### [05385] Asset Bubble Riding with Price-Dependent Entry: a Mean Field Game of Controls with Common Noise

**Author(s) :** Dylan Possamai (ETH Zürich)Shichun Wang (Princeton University)

**Abstract :** In this talk, we present an existence result for mean field games of controls with common noise and random entry time. We obtain an equilibrium by first solving discretized versions of the game in the weak formulation and examining the measurability property in the limit. As a motivating example, we extend the existing game-theoretic model on optimal execution in the presence of an asset bubble by allowing for price-dependent entry times. Agents are characterized by their individual entry thresholds that represent their beliefs in the strength of the bubble. Conversely, the growth dynamics of the bubble is fueled by the influx of players. On top of the asset price, a second source of common noise is the exogenous bubble burst time, which we incorporate into the model via progressive enlargement of filtration. In the end, we show the equilibrium strategy can be decomposed into before-and-after-burst segments, each part containing only the market information.

### [05410] Bubble Riding with Price-Dependent Entry: Mean Field Games of Controls with Common Noise

**Author(s) :** Ludovic Tangpi (Princeton University)Shichun Wang (Princeton University)

**Abstract :** In this talk, we present an existence result for mean field games of controls with common noise and random entry time. We obtain an equilibrium by first solving discretized versions of the game in the weak formulation and examining the measurability property in the limit. As a motivating example, we extend the existing game-theoretic model on optimal execution in the presence of an asset bubble by allowing for price-dependent entry times. Agents are characterized by their individual entry thresholds that represent their beliefs in the strength of the bubble. Conversely, the growth dynamics of the bubble is fueled by the influx of players. On top of the asset price, a second source of part\_1

common noise is the exogenous bubble burst time, which we incorporate into the model via progressive enlargement of filtration. In the end, we show the equilibrium strategy can be decomposed into before-and-after-burst segments, each part containing only the market information.

## [00151] Recent trends in SHM: damage modeling and optimal experimental design from a mechanical and mathematical point of view

### **Session Time & Room :**

00151 (1/2) : 4C (Aug.24, 13:20-15:00) @F403

00151 (2/2) : 4D (Aug.24, 15:30-17:10) @F403

**Type :** Proposal of Minisymposium

**Abstract :** Structural and mechanical systems like bridges, buildings and defense systems play an essential role in modern societies. The maintenance of these structures must provide their safety and prevent the loss of life but at the same time be cost-efficient. Usually, the monitoring issue has been tackled from an engineering point of view. Consequently, the number of possible problem-solving algorithms is drastically reduced. In this minisymposium, the approaches from a mathematical and mechanical point of view are presented. These lead from methods for optimal sensor placements and applications of shape optimization to numerical simulations of damage detection, evolution, and prognosis.

**Organizer(s) :** Kathrin Welker, Natalie Rauter

**Classification :** 49Q10, 74J25, 74M25, 74P10, 74R99

### **Minisymposium Program :**

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00151 (1/2) : 4C @F403 [Chair: Kathrin Welker]

## [00271] Optimization aspects of experimental design approaches for sensor placement

**Format :** Talk at Waseda University

**Author(s) :** Volker Schulz (Trier University)

**Abstract :** The information from sensors has to be treated in order to obtain properties of technical systems. The accuracy expressed in statistical concepts like covariance matrix and confidence regions depends on constituents of the measurement process. This talk discusses the effect of sensor placement and actuator design on these statistical properties and presents mathematical optimization approaches to optimize them.

## [00272] Fracture propagation by using shape optimization techniques on Riemannian spaces

**Format :** Talk at Waseda University

**Author(s) :** Tim Suchan (Helmut Schmidt University/University of the Federal Armed Forces Hamburg)Kathrin Welker (TU Bergakademie Freiberg)Winnifried Wollner (University of Hamburg)

**Abstract :** The concept of smooth phase fields has been used successfully to predict fracture propagation. However, it usually requires minimum two regularization parameters to be tuned. We present a novel approach for numerical fracture simulation which avoids the usage of phase fields. Instead, an objective functional that drives the evolution of the fracture is minimized with shape optimization techniques. We present the mathematical approach and numerical results for various commonly-used benchmarks.

## [00246] Numerical modeling of crack propagation in concrete by means of cohesive zone modeling and a novel phase-field fracture approach

**Format :** Talk at Waseda University

**Author(s) :** Rasoul Najafi Koopas (Helmut-Schmidt University)

**Abstract :** Two methodologies are developed for analyzing failure initiation and crack propagation in the highly inhomogeneous concrete mesostructure. By implementing efficient algorithms in Python, geometric features are

generated and packed into a continuous phase. In the case of concrete, the continuous phase represents the mortar matrix, while the geometric features are the aggregates and voids of different sizes distributed randomly within the mortar matrix to represent the complex two-dimensional mesostructures of the concrete. The failure initiation and crack propagation of mesoscale concrete specimens are investigated using two different approaches, namely the Cohesive Zone Model and a novel Phase-Field fracture model. In the first approach, crack propagation is realized by generating zero-thickness Cohesive Interface Elements at the interfaces of solid elements. For this purpose, two-dimensional cohesive interface elements are generated (*i*) within the constituent elements of the mortar matrix, (*ii*) within the elements constituting the aggregates, and (*iii*) at the Interfacial Transition Zone. Hence, all potential crack paths are simulated by assigning different Traction Separation laws to the cohesive interface elements generated in different regions of the mesoscale concrete specimen. In the second approach, a novel cohesive phase-field is developed by incorporating the idea proposed by Wu and Nguyen (2018) and Geelen et al. (2019) in which by a group of optimal characteristic functions, a phase-field regularized cohesive zone model with linear softening law is realized and applied to brittle fracture. Moreover, the implemented cohesive phase-field fracture is insensitive to the length scale parameter, which allows the use of a relatively coarser mesh, thereby significantly reducing the computational cost [3]. A series of mesoscale concrete specimens with identical properties (*volumedensity, sizedistribution, and aggregate shape*) are simulated using the above approaches and the predicted crack paths are compared with each other.

#### References:

- 1- Wu, Jian-Ying, and Vinh Phu Nguyen. "A length scale insensitive phase-field damage model for brittle fracture." Journal of the Mechanics and Physics of Solids 119 (2018): 20-42.
- 2- Geelen, Rudy JM, et al. "A phase-field formulation for dynamic cohesive fracture." Computer Methods in Applied Mechanics and Engineering 348 (2019): 680-711.
- 3- Rezaei, Shahed, et al. "An anisotropic cohesive fracture model: Advantages and limitations of length-scale insensitive phase-field damage models." Engineering Fracture Mechanics 261 (2022): 108177.

## [00231] Sequential subspace optimization for recovering stored-energy functions in hyperelastic materials

**Format :** Talk at Waseda University

**Author(s) :** Lukas Vierus (Saarland University)Rebecca Rothermel (Saarland University)Thomas Schuster (Saarland University)Anne Wald (University of Göttingen)

**Abstract :** Structural Health Monitoring demands for an efficient computation of parameters which characterize the mechanical behavior of elastic materials. Hyperelasticity describes a nonlinear elastic behavior where the second Piola-Kirchhoff stress tensor is given as a derivative of a scalar function representing the stored strain energy that encodes all mechanical properties of the underlying material. The mathematical model is represented by a high-dimensional parameter identification problem for a nonlinear, hyperbolic system with given initial and boundary values. We present an iterative method based on sequential subspace optimization leading to a significant acceleration compared to the Landweber method.

00151 (2/2) : 4D @F403 [Chair: Natalie Rauter]

## [00230] A low power autonomous SHM node for aerospace applications

**Format :** Talk at Waseda University

**Author(s) :** Carol Featherston (School of Engineering, Cardiff University)Rhys Pullin (School of Engineering, Cardiff University)Stephenn Griggs (School of Engineering, Cardiff University)Matthew Pearson (School of Engineering, Cardiff University)

**Abstract :** Acoustic emission(AE) monitors the release of energy resulting from the growth of damage to determine structural integrity. It is difficult to apply in low-power systems as sensors must either be wired together or time synchronised, which is power intensive. A method based on three piezoelectric sensors in a small triangular array is proposed. Hardware is developed and the feasibility of powering the unit through energy harvesting explored. Results are obtained for a complex composite structure.

## [00270] Damage parameter estimation in composite materials using data assimilation with reduced order models

**Format :** Online Talk on Zoom

**Author(s) :** Nanda Kishore Bellam Muralidhar (TU Braunschweig)Carmen Gräßle (TU Braunschweig)Natalie Rauter (HSU Hamburg)Rolf Lammering (HSU Hamburg)Andrey Mikhaylenko (HSU Hamburg)Dirk Lorenz (TU Braunschweig)

**Abstract :** In this work, we are concerned with estimating parameters that describe damage in composite materials. In particular, we consider fiber metal laminates which consist of metals and fiber reinforced plastics. Such materials are of great interest in e.g. aviation and automotive industries. We study structural health monitoring using guided ultrasonic waves utilizing an integrated sensor. In order to determine the damage parameters, we use techniques from Bayesian

inference and data assimilation together with model order reduction which enables to alleviate the computational efforts. Numerical simulations illustrate the approaches.

## [00256] Coefficient Control for Variational Inequalities

**Format :** Talk at Waseda University

**Author(s) :** Nicolai Simon (Universität Hamburg)Winnifried Wollner (Universität Hamburg)

**Abstract :** We consider the effects of introducing a control variable into the coefficients of a variational inequality in an optimal control problem with complementarity constraints.

The novelty of this talk is the utilization of H-convergence methods to formulate limit arguments as the basis for a bootstrapping approach, used to prove strong  $L^p$  convergence of the coefficient control variable. Using the example of an obstacle problem, we compute a set of limiting optimality conditions using these arguments.

## [00269] Optimal sparse sensor location for structural health monitoring

**Format :** Online Talk on Zoom

**Author(s) :** Olga Weiß (Helmut Schmidt University/ University of the Federal Armed Forces Hamburg)Kathrin Welker (TU Bergakademie Freiberg)Volker Schulz (Trier University)

**Abstract :** Bridge structures are indispensable components of the infrastructure of modern industrial societies, and maintaining their functionality and reliability is essential.

Hence, monitoring processes of the structure and health of bridges are indispensable. For this purpose, the efficient and optimal placement of appropriate sensors for the non-destructive permanent monitoring of the structures is an important component.

Determining the number and placement of sensors to provide valuable information about damage and impact to the structure is essential for cost-efficient monitoring and for minimizing the volume of data, however, to this date represents a challenge.

We consider this issue from a mathematical point of view and derive a suitable optimization problem in infinite-dimensional function spaces. This modeled optimization problem is to be solved numerically by adapted optimization methods. As a special feature, the desired resulting sparsity of the solution for the positioning of the sensors is to be incorporated and considered in the solving method.

## [00153] Recent Advances on Inverse Analysis

**Session Time & Room :** 1E (Aug.21, 17:40-19:20) @E811

**Type :** Proposal of Minisymposium

**Abstract :** In inverse analysis, unknown design variables and parameters are calculated so as to satisfy observed values and design standard values, and this kind of analysis is widely performed in design problems, i.e., shape optimization and topology optimization problems, and parameter identification problems. The adjoint variable method, the direct differentiation method, the Kalman filter, etc. are generally employed to solve these problems. However, the solution may not be appropriately calculated unless special methods are used. In this mini symposium, the purpose is to discuss new numerical methods and considerations to solve problems in inverse analysis.

**Organizer(s) :** Takahiko Kurahashi, Jin-Xing Shi, Masayuki Kishida, Eiji Katamine

**Classification :** 74P05, 65K10, 37N10, 74F10, Inverse Analysis

**Minisymposium Program :**

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00153 (1/1) : 1E @E811 [Chair: Takahiko Kurahashi]

## [01421] Tidal current estimation based on the extended Kalman filter FEM

**Format :** Talk at Waseda University

**Author(s) :** Takahiko Kurahashi (Nagaoka University of Technology)

**Abstract :** In this presentation, some numerical results of tidal current estimation analysis for Tokyo bay model will be shown. The shallow water equation is introduced as the governing equation, and the discretized equation is employed as the system equation in the extended Kalman filter FEM. Numerical results will be compared with the result based on the normal Kalman filter FEM, and the superiority of extended Kalman filter FEM will be shown.

## [01427] Optimal shape design of auxetic structures with periodicity

**Format :** Talk at Waseda University

**Author(s) :** Jin-Xing Shi (Komatsu University)

**Abstract :** Auxetic structures indicate structures with negative Poisson's ratio. To achieve their best auxetic performance, in this work, optimal shape design of periodic auxetic structures is performed for identification of the negative Poisson's ratio based on a gradient-based shape optimization method and the homogenization method. Numerical design examples are given to confirm the validity and efficiency of the proposed optimization approach. The present work aims to help design auxetic structures in industrial applications.

## [01428] Density-based topology optimization using a modified optimality criteria method

**Format :** Online Talk on Zoom

**Author(s) :** Masayuki Kishida (National Institute of Technology (KOSEN), Gifu College)Takahiko Kurahashi (Nagaoka University of Technology)

**Abstract :** In this study, we present the density-based topology optimization for minimizing equivalent stress using our developed modified optimality criteria method. The method is an update method for density that incorporates the concepts of Newton's method for the conventional optimality criteria method. The number of arbitrary constants required for topology optimization can be reduced by using our proposed method. In this presentation, p-norm is employed for the performance function and several numerical results will be presented.

## [03034] Shape Design Problems Considering Fluid-Structure-Interactive Fields

**Format :** Talk at Waseda University

**Author(s) :** Eiji Katamine (National Institute of Technology, Gifu College)Yashushi Yoshida (Gifu University)

**Abstract :** This paper presents numerical solution to a shape design of stationary fluid-structure-interactive fields. The minimization problem for total dissipation energy in the viscous flow field and the mean compliance minimization problem in order to achieve stiffness maximization in the structural field are considered for the shape optimization. Numerical analysis program for the shape design is developed by using FreeFEM, and the validity of proposed method is confirmed by results of 2D numerical analyses.

## [00154] Homogenization of PDEs in domains with oscillating boundaries or interfaces

**Session Time & Room :**

00154 (1/2) : 2D (Aug.22, 15:30-17:10) @F312

00154 (2/2) : 2E (Aug.22, 17:40-19:20) @F312

**Type :** Proposal of Minisymposium

**Abstract :** Homogenization is a mathematical way of understanding microscopic structure via macroscopic medium and hence has enormous applications in science and engineering fields, including material science, as heat diffusion, fluid flows, deformations, and biological applications as electrical conduction in tissues like nerve or heart fibers. In this symposium, we consider two types of closely related homogenization problems: complex domains consisting of a fixed part and a rapidly oscillating part, and domains with oscillating interfaces with jump-conditions.

The aim of this minisymposium is to present recent results in these two important subjects by known specialists worldwide, and allow discussions opening new directions.

**Organizer(s) :** Patrizia Donato, Akambadath K. Nandakumaran

**Classification :** 35B27, 74A50, 74KXX, 76M50, 35BXX

**Minisymposium Program :**

00154 (1/2) : 2D @F312 [Chair: Patrizia Donato]

## [00392] Asymptotic analysis of a parabolic problem with a rough fast oscillating interface

**Format :** Talk at Waseda University

**Author(s) :** Patrizia Donato (Univ Rouen Normandie, France) Editha Carreon Jose (University of the Philippines Los Banos) Daniel Onofrei (University of Houston)

**Abstract :** In this talk, we will discuss the well posedness and prove several homogenization results for a parabolic problem with an imperfect contact on the rough fast oscillating interface separating a domain occupied by heterogeneous materials. The complexity of the domain geometry and the imperfect contact on the interface create interesting multiscale phenomena with different macroscale behaviors depending on model parameters.

## [00417] A decomposition result for thin domains with rough boundary

**Format :** Talk at Waseda University

**Author(s) :** Juan Casado-Díaz (University of Seville) Manuel Luna-Laynez (University of Seville) Francisco Javier Suárez-Grau (University of Seville)

**Abstract :** We prove a decomposition result for the pressure of a fluid in a thin domain. This result extends to the linear elasticity framework, providing better estimates for the Korn constant and fine decompositions for the elastic deformations. We show how these results, which give additional compactness properties, apply to study the asymptotic behaviour of some problems in fluid mechanics and elasticity, posed in thin domains with rough boundaries.

## [00412] Derivation of coupled Stokes-Plate-Equations for fluid flow through thin porous elastic layers

**Format :** Online Talk on Zoom

**Author(s) :** Maria Neuss-Radu (Friedrich-Alexander-Universität Erlangen-Nürnberg) Markus Gahn (University Heidelberg) Willi J"ager (University Heidelberg)

**Abstract :** We consider two fluid-filled bulk domains separated by a thin porous elastic layer with thickness and periodicity  $\epsilon$ . The fluid flow is described by an instationary Stokes-system, and the solid via linear elasticity. By rigorous homogenization and dimension reduction methods, we derive for  $\epsilon \rightarrow 0$  an effective model consisting of the Stokes-equations in the bulk domains coupled to a time dependent plate equation with homogenized coefficients on the effective interface separating the bulk regions.

## [00416] Homogenization of a two-component domain with an oscillating thick interface

**Format :** Online Talk on Zoom

**Author(s) :** Klas Pettersson (Freelance) Patrizia Donato (Univ Rouen Normandie, France)

**Abstract :** The homogenization of an elliptic boundary value problem is considered in a finite cylindrical domain that consists of two components separated by a periodically oscillating thick interface. On the interface, the flux is assumed to be continuous, and the jump of the solution to be proportional to the flux through the interface. By means of the periodic unfolding method, we derive the homogenized system, and prove the convergence of the solutions and their energies.

00154 (2/2) : 2E @F312 [Chair: Akambadath K. Nandakumaran]

## [00402] Heat conduction in composite media involving imperfect contact conditions

**Format :** Online Talk on Zoom

**Author(s) :** Micol Amar (Sapienza Università di Roma) Daniele Andreucci (Sapienza Università di Roma) Claudia Timofte (University of Bucharest)

**Abstract :** We present a model which exhibit simultaneously jumps in the solution and in the flux, involving also the mean average of the physical fields representing the different phases. The starting model is a composite made by a hosting medium containing a periodic array of inclusions of small size, coated by a thin layer made by two different materials, one encapsulated in the other. The smallness of the thin layer leads us to perform first a two-step concentration procedure. The periodic structure leads to a homogenization limit, in order to achieve a macroscopic description.

## [00399] Homogenization by unfolding of a Bingham fluid in a thin domain with rough boundary

**Format :** Online Talk on Zoom

**Author(s) :** Carmen Perugia (Department of Science and Technology, University of Sannio)Manuel Villanueva-Pesqueira (Universidad Pontificia Comillas)Giuseppe Cardone (University of Naples "Federico II")

**Abstract :** We consider a Bingham flow in a thin domain with rough boundary and with no-slip boundary condition on the whole boundary of the domain. By using an adapted linear unfolding operator we perform a detailed analysis of the asymptotic behavior of the Bingham flow when thickness of the domain and roughness periodicity tends to zero. We obtain the homogenized problem for the velocity and the pressure, which preserves the nonlinear character of the flow.

## [00401] Homogenization of Stokes system with Neumann condition on highly oscillating boundary

**Format :** Talk at Waseda University

**Author(s) :** Bidhan Chandra Sardar (Indian Institute of Technology Ropar)

**Abstract :** We consider the steady Stokes system in a  $n$ -dimensional domain  $\Omega_\varepsilon$  with a rapidly oscillating ( $n - 1$ ) dimensional boundary prescribed with Neumann boundary condition and periodicity along the lateral sides is considered. We aim to study the limiting analysis (as  $\varepsilon \rightarrow 0$ ) of the steady Stokes problem and identify the limit problem in a fixed domain. Finally, show the weak convergences of velocities are improved to strong convergence by introducing corrector terms.

## [00407] Fluids with a non-slip condition on a non-periodic oscillating boundary

**Format :** Talk at Waseda University

**Author(s) :** Juan Casado-Díaz (University of Seville)Manuel Luna-Laynez (University of Seville)

**Abstract :** It is known that a viscous fluid with a non-slip condition on a rough boundary behaves as if an adherence condition is imposed. This is the case for a boundary given by  $x_3 = \delta_\varepsilon \psi(x_1/\varepsilon, x_2/\varepsilon)$ ,  $\psi$  periodic, and  $\delta_\varepsilon/\varepsilon^{3/2}$  tending to infinity. The rugosity has not effect if it tends to zero. In the critical case a new zero order term appears in the boundary condition. Here, we extend these results to non-periodic boundaries.

# [00164] Recent Advances in Direct and Inverse Problems in Mathematical Materials Science

**Session Time & Room :**

00164 (1/3) : 2C (Aug.22, 13:20-15:00) @G801

00164 (2/3) : 2D (Aug.22, 15:30-17:10) @G801

00164 (3/3) : 2E (Aug.22, 17:40-19:20) @G801

**Type :** Proposal of Minisymposium

**Abstract :** In recent years, there has been a tremendous growth of activity in developing methods for materials-related phenomena occurring over multiple scales in time and space. This minisymposium focuses on multiscale modeling, analysis, and simulation of the problems arising in composites and other heterogeneous media. In particular, topics that will be discussed include but are not limited to asymptotic analysis such as homogenization, modeling of new materials, inverse problems, and computational tools. The purpose of this minisymposium is to encourage the exchange of ideas and networking among researchers working on the topics mentioned above.

**Organizer(s) :** Lyudmyla Barannyk, Silvia Jimenez Bolanos, Yvonne Ou  
**Sponsor :** This session is sponsored by the SIAM Activity Group on Mathematical Aspects of Materials Science.

**Classification :** 35Qxx, 74Qxx, 74Rxx, 80Axx, 78Mxx

**Minisymposium Program :**

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00164 (1/3) : 2C @G801 [Chair: Lyudmyla Barannyk]

## [00473] Bloch Waves in High Contrast Electromagnetic Crystals

**Author(s)** : Silvia Jimenez Bolanos (Colgate University)Robert Lipton (Louisiana State University)Robert Viator (Swarthmore College)Abiti Adili (University of Massachusetts Lowell)

**Abstract** : In this talk, we present the derivation of analytic representation formulas and power series describing the band structure inside non-magnetic periodic photonic crystals, made from high dielectric contrast inclusions. We identify a resonance spectrum for quasi-periodic source-free modes, which are used to represent solution operators associated with electromagnetic and acoustic waves inside periodic high-contrast media. A convergent power series for the Bloch wave spectrum is obtained from the representation formulas and explicit conditions on the contrast are found that provide lower bounds on the convergence radius. These conditions are sufficient for the separation of spectral branches of the dispersion relation for any fixed quasi-momentum.

## [00483] An axisymmetric problem for a nano-sized material surface on a boundary of an elastic semi-space

**Author(s)** : Anna Zemlyanova (Kansas State University)

**Abstract** : An axisymmetric problem for a nano-sized penny-shaped material surface attached to the boundary of an elastic isotropic semi-space is considered. The surface is modeled using the Steigmann-Ogden form of surface energy. The problem is solved by using the Boussinesq potentials and Hankel transforms. The problem can be reduced to a system of two singular integral equations. This is a joint work with Lauren M. White.

## [00569] Clusters of Bloch waves in three-dimensional periodic media

**Author(s)** : Yuri Godin (University of North Carolina at Charlotte)

**Abstract** : We consider acoustic wave propagation through a periodic array of small inclusions of arbitrary shape. The inclusion size is much smaller than the array period while the wavelength is fixed. We derive and rigorously justify the dispersion relation for general frequencies and show that there are exceptional frequencies for which the solution is a cluster of waves propagating in different directions with different frequencies so that the dispersion relation cannot be defined uniquely. The results are illustrated by an example of a medium with a simple cubic lattice of spherical inclusions where we derived the dispersion relation, determine the parameters of the effective medium, and provided examples of some clusters. This is joint work with B. Vainberg.

## [00588] Modeling sea ice as a multiscale composite material

**Author(s)** : Kenneth Morgan Golden (University of Utah)

**Abstract** : Sea ice exhibits composite structure on length scales ranging over many orders of magnitude. Forward and inverse homogenization are central to modeling sea ice and its role in climate and ecosystems. We'll tour recent advances, from the fractal geometry of millimeter-scale brine inclusions and meter-scale melt ponds, to the homogenized dynamics of the marginal ice zone on the scale of the Arctic Ocean. We'll also explore spectral representations for effective parameters in several contexts.

00164 (2/3) : 2D @G801 [Chair: Yvonne Ou]

## [00596] Forward and inverse homogenization for quasiperiodic composites

**Author(s)** : Elena Cherkaev (University of Utah)Sébastien Guenneau (Imperial College London)Niklas Wellander (Swedish Defence Research Agency )

**Abstract** : From quasicrystalline alloys to twisted bilayer graphene, materials with a quasiperiodic structure exhibit unusual properties that drastically differ from those with periodic structures. Quasiperiodic geometries can be modeled using the cut-and-projection method restricting a periodic function in a higher-dimensional space to a lower-dimensional subspace cut at an irrational projection angle. The talk will discuss the homogenized equations for quasiperiodic materials and an inverse problem of recovering information about microstructural parameters from known effective properties.

## [00609] Studying Stefan problems with internal heat generation using sharp interface models

**Format** : Talk at Waseda University

**Author(s)** : Lyudmyla L. Barannyk (University of Idaho)John C. Crepeau (University of Idaho)Patrick Paulus (University of Idaho)Alexey Sakhnov (Kutateladze Institute of Thermophysics SB RAS)Sidney D. V. Williams (Georgia Institute of Technology)

**Abstract** : We study the evolution of the solid-liquid interface during melting and solidification of a material with constant internal heat generation with prescribed temperature and heat flux conditions at the boundary of an infinite

cylinder. We derive a nonlinear differential equation for the motion of the interface, which involves Fourier-Bessel series. The problem is also solved numerically by the front catching into a space grid node method as well as the enthalpy-porosity method to validate results.

### [00623] Capturing Quasistatic Fracture Evolution with Nonlocal Models

**Author(s)** : Robert Lipton (Louisiana State University)Debdeep Bhattacharya (Louisiana State University)

**Abstract** : Nonlocal quasistatic fracture evolution for interacting cracks is developed. The approach is implicit and based on local stationarity and fixed point methods. It is proved that the fracture evolution decreases the stored elastic energy with each load step; provided the load increments are taken sufficiently small. Existence theory for the fracture evolution is proved rigorously. Numerical examples include capturing the crack path propagating inside an L-shaped domain, and two offset inward propagating cracks.

### [00631] The Lippmann-Schwinger Lanczos algorithm for inverse scattering problems

**Author(s)** : Shari Moskow (Drexel University)Vladimir Druskin (WPI)Mikhail Zaslavsky (Southern Methodist University)

**Abstract** : We combine data-driven reduced order models with the Lippmann-Schwinger integral equation to produce a direct nonlinear inversion method. The ROM is viewed as a Galerkin projection and is sparse due to Lanczos orthogonalization. Embedding into the continuous problem, a data-driven internal solution is produced. This internal solution is then used in the Lippmann-Schwinger equation, in a direct or iterative framework. The approach also allows us to process more general transfer functions, i.e., to remove the main limitation of the earlier versions of the ROM based inversion algorithms. We also describe how the generation of internal solutions simplifies in the time domain and give examples of its use given mono static data, targeting synthetic aperture radar.

00164 (3/3) : 2E @G801 [Chair: Silvia Jimenez Bolanos]

### [00647] Uncertainty quantification for stochastic models of damage mechanics

**Author(s)** : Petr Plechac (University of Delaware)Gideon Simpson (I University)Jerome R Troy (University of Delaware)

**Abstract** : We study models used for describing brittle materials which exhibit linear elastic behavior until an applied load reaches a critical yield stress at which point a damage/fracture occurs. The underlying visco-elasto dynamics PDEs are characterized by a non-monotone stress-strain relation with a non-linearity linked to the critical yield stress. We study these equations in the presence of random yield stress field. The developed computational techniques will be demonstrated in numerical examples.

### [00649] On the governing equations of poro-piezoelectric composite materials

**Author(s)** : Miao-Jung Yvonne Ou (University of Delaware)

**Abstract** : Materials such as quartz, cortical bones and cancellous bones exhibit piezo-electric behaviors, for which a mechanical wave such as ultrasound can trigger electro-magnetic waves. In this talk, we consider a porous material made of piezo-electric solid with pores saturated with conducting fluid, a model mimicking *in vivo* bones. The focus is to understand how the microstructure is encoded in the effective piezoelectric properties of these porous composites by using the two-scale convergence homogenization approach.

### [01237] Homogenization of a suspension of viscous fluid with magnetic particles

**Author(s)** : Yuliya Gorb (NSF)Thuyen Dang (University of Chicago)Silvia Jimenez Bolanos (Colgate University)

**Abstract** : In this talk, the rigorous periodic homogenization for a coupled system, which models a suspension of magnetizable rigid particles in a non-conducting carrier viscous Newtonian fluid is discussed. Both one-way and two-way coupling between the fluid and particles are considered. As the size of the particles approaches zero, it is shown that the suspension's behavior is governed by a generalized homogenized magnetohydrodynamic system, whose parameters are explicitly derived. The two-scale convergence is utilized to justify obtained homogenized behavior of the original heterogeneous system.

## [05177] Energy-efficient flocking of particle systems

**Author(s)** : Alexander Panchenko (Washington State University)

**Abstract** : The talk explores the problem of achieving flocking in multi-agent systems using minimal amount of on-board energy.

We also assume that censor capacity is limited. Starting from a model reminiscent of Dissipative Particle Dynamics augmented with self-propulsion forces, we prove existence of an attractor for certain non-dissipative systems. Computer simulations show that velocity alignment is more energy efficient than formation control.

## [00168] Applications of evolutionary algorithms in differential equation models

**Session Time & Room :**

00168 (1/2) : 1C (Aug.21, 13:20-15:00) @E811

00168 (2/2) : 1D (Aug.21, 15:30-17:10) @E811

**Type** : Proposal of Minisymposium

**Abstract** : Evolutionary algorithms (EAs) have been at the forefront of computational science in solving optimization problems arising from science and engineering. EAs gained popularity because of their capability to obtain global minimizers of non-smooth objective functions. In this minisymposium, we explore the applications of EAs in solving optimization problems arising from differential equation models. Recent techniques in unconstrained, constrained, and multi-objective EAs will be presented along with applications in parameter estimation and control of infectious disease models, medical image reconstruction in electrical impedance tomography, optimal placement of sensors of tsunami sensors, and other applications in engineering.

**Organizer(s)** : Renier Mendoza, Eunok Jung

**Classification** : 68W50, 90C26, 34H05, 35R30, 92-10

**Minisymposium Program :**

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00168 (1/2) : 1C @E811

## [03121] Spherical search with multi-operator differential evolution for constrained optimization problems

**Format** : Talk at Waseda University

**Author(s)** : Renier Mendoza (Institute of Mathematics, University of the Philippines Diliman)Jongmin Lee (Konkuk University)Victoria May Paguio Mendoza (University of the Philippines Diliman)Eunok Jung (Konkuk University)

**Abstract** : We propose a new method, SASS-MODE, for solving constrained optimization problems by combining the self-adaptive spherical search (SASS) with the improved multi-operator differential evolution (IMODE). We adapted IMODE to handle constraints with three modifications and tested our method on 57 benchmark problems and an optimal control problem from an infectious disease model. SASS-MODE outperforms recent algorithms and achieves state-of-the-art results.

## [02925] Minimizing infections and intervention cost: multi-objective approach with user-friendly dashboard

**Format** : Talk at Waseda University

**Author(s)** : Jongmin Lee (Department of Mathematics, Konkuk University)Renier Mendoza (Institute of Mathematics, University of the Philippines Diliman)Victoria May P. Mendoza (Institute of Mathematics, University of the Philippines Diliman)Eunok Jung (Department of Mathematics, Konkuk University)

**Abstract** : During the COVID-19 pandemic, the world faces the challenge of reducing the number of infections while simultaneously minimizing the cost of intervention policies. This study proposes a deterministic model and multi-objective optimization approach that balances these conflicting objectives. Metropolis-Hastings algorithm estimated parameters, and the genetic algorithm found multi-objective optimization solutions. From Pareto solutions, users can select the most suitable solution by considering economic-related parameters. Additionally, we develop a user-friendly, web-based dashboard for ease of use.

## [02755] Comparative Study of Heuristic Algorithms for Electrical Impedance Tomography

**Format :** Talk at Waseda University

**Author(s) :** Arrianne Crystal Velasco (Institute of Mathematics, University of the Philippines Diliman)Renier Mendoza (Institute of Mathematics, University of the Philippines Diliman)Marion Darbas (LAGA CNRS UMR 7539, University Sorbonne Paris Nord)Monica Bacon (Institute of Mathematics, University of the Philippines Diliman)John Cedrick de Leon (Institute of Mathematics, University of the Philippines Diliman)

**Abstract :** Based on electrical measurements from electrodes placed around the boundary of a body, electrical impedance tomography (EIT) is an imaging procedure that recovers the spatial distribution of the conductivities in the interior of a body. This work presents a study of the applicability of six heuristic algorithms for the EIT image reconstruction problem.

## [03163] Bi-objective optimization considering bed capacity and timing of interventions

**Format :** Talk at Waseda University

**Author(s) :** Victoria May Paguio Mendoza (University of the Philippines Diliman)Renier Mendoza (Institute of Mathematics, University of the Philippines Diliman)Youngsuk Ko (Department of mathematics, Konkuk university)Jongmin Lee (Konkuk University)Eunok Jung (Konkuk University)

**Abstract :** Without vaccines and medicine, non-pharmaceutical interventions are the main strategy for controlling the spread of diseases. A bi-objective optimization problem is formulated that allows for the easing of restrictions at an earlier time and minimizes the number of additional beds ensuring sufficient capacity in healthcare facilities. We utilize a compartmental model that distinguishes mild from severe cases. The multiple optimal solutions of the bi-objective problem offer trade-off solutions that can be useful decision-support tools.

00168 (2/2) : 1D @E811 [Chair: Arrianne Crystal Velasco]

## [00170] Integrable systems, orthogonal polynomials and asymptotics

**Session Time & Room :**

00170 (1/3) : 2C (Aug.22, 13:20-15:00) @G401

00170 (2/3) : 2D (Aug.22, 15:30-17:10) @G401

00170 (3/3) : 2E (Aug.22, 17:40-19:20) @G401

**Type :** Proposal of Minisymposium

**Abstract :** Interest in nonlinear dynamical systems has grown dramatically over the past half century. Profound advances have been fueled by the discovery of integrable systems that are applicable in a wide range of applications. In particular, nonlinear ODEs called the Painlevé' equations model applications in many fields, in particular in random matrix theory and growth processes. Their appearance in quantum gravity and orthogonal polynomial theory has led to widening interest in integrable discrete versions of these equations. This minisymposium will bring together recent developments in integrable systems, orthogonal polynomials and asymptotics with a view to describing new special functions.

**Organizer(s) :** Nalini Joshi, Nobutaka Nakazono, Milena Radnovic, Da-jun Zhang,

**Classification :** 33E17, 33C45, 41A60

**Minisymposium Program :**

00170 (1/3) : 2C @G401 [Chair: Da-jun Zhang]

## [05493] Welcome and Introduction

**Format :** Talk at Waseda University

**Author(s) :** Nalini Joshi (The University of Sydney)

**Abstract :** This talk will provide an overview of recent developments in integrable systems, orthogonal polynomials and asymptotics and the topics underlying the talks in this minisymposium.

## [02937] Lagrangian multiform structure of discrete and semi-discrete KP typequations

**Format :** Talk at Waseda University

**Author(s) :** Frank Willem Nijhoff (University of Leeds)

**Abstract :** A brief review of of Lagrangian multiform theory for integrable discrete and continuous equations will be presented. As specific examples I will discuss the recently established 3-form structure of the KP hierarchy, and its discrete and semi-discrete counterparts.

## [03500] Charge-conserving solutions to the constant Yang-Baxter equations

**Format :** Talk at Waseda University

**Author(s) :** Jarmo Hietarinta (University of Turku)Paul Martin (University of Leeds)Eric C. Rowell (Texas A&M University)

**Abstract :**

The Yang-Baxter equation is difficult to solve even in the constant form  $R_{12}R_{13}R_{23} = R_{23}R_{13}R_{12}$  and a complete solution is known only for rank two. For further progress it is important to make a meaningful ansatz. Recently Martin and Rowell proposed charge-conservation as an effective constraint (arXiv:2112.04533). We explore the results obtained by a slightly different charge-conservation rule.

## [03983] Stokes' phenomenon, discretization, and discrete integrability

**Format :** Talk at Waseda University

**Author(s) :** Christopher Lustri (Macquarie University)

**Abstract :** This talk is concerned with integrability in discrete systems, and its relationship with Stokes' phenomenon. Discrete equations such as the discrete Painlevé I equation can be written in terms of an infinite-order differential equation. We will consider a family of equations obtained by truncating this infinite-order differential equation at different orders. In this talk we will answer two questions: (1) How does discretization connect the Stokes' phenomenon in continuous and discrete Painlevé I? (2) How does integrability emerge in this family of equations in the discrete limit?

00170 (2/3) : 2D @G401 [Chair: Nalini Joshi]

## [04872] On q-Painlevé VI and the geometry of affine Segre surfaces

**Format :** Talk at Waseda University

**Author(s) :** Pieter Roffelsen (University of Sydney)

**Abstract :** A famous result by M. Jimbo (1982) relates Painlevé VI to a family of affine cubic surfaces via the Riemann-Hilbert correspondence. In recent work with Nalini Joshi, a  $q$ -analog of this result was obtained, relating  $q$ -Painlevé VI to a family of affine Segre surfaces. I will explain this result and show how the geometry of these surfaces is reflected in the asymptotic expansions of solutions around the two critical points of  $q$ -Painlevé VI.

## [04990] Deformed orthogonal functions and integrable lattices

**Format :** Talk at Waseda University

**Author(s) :** Xiangke Chang (Academy of Mathematics and Systems Science, Chinese Academy of Sciences)

**Abstract :** Since the 1990s, the theory of orthogonal polynomials has been increasingly playing an important role in the studies of Toda type lattices, peakon dynamical systems of the Camassa-Holm type, as well as specific Painlevé equations. These integrable lattices can be derived according to deformations of orthogonal functions, directly or indirectly. This talk is devoted to exploring some of related works with focus on our recent results for some new orthogonality.

## [05269] Borel analysis for the first difference q-Painlevé equation

**Format :** Talk at Waseda University

**Author(s) :** Adri Olde Daalhuis (The University of Edinburgh)

**Abstract :** We discuss the asymptotics of solutions of the first -difference  $q$ -Painlevé equation  $w(gt)w^2(t)w(t/q) = w(t) - t$ . Via the  $q$ -Borel transform we obtain an interesting singularity distribution in the Borel plane.

## [05326] Non-linear Stokes phenomenon for Painleve transcedents and topological recursion

**Format :** Talk at Waseda University

**Author(s) :** Kohei Iwaki (The University of Tokyo)

**Abstract :** I will propose a conjectural statement on the Stokes phenomenon for the topological recursion partition function. Our claim is based on a relation between the topological recursion and the Painleve tau-function through the exact WKB analysis.

00170 (3/3) : 2E @G401 [Chair: Nobutaka Nakazono]

## [05494] Orthogonal polynomials on elliptic curves and Painlevé VI equation.

**Author(s) :** Harini Desiraju (University of Sydney)Pieter Roffelsen (University of Sydney)Tomas Latimer (University of Sydney)

**Abstract :** Elliptic orthogonal polynomials are a family of special functions that satisfy certain orthogonality condition with respect to a weight function on an elliptic curve. Building up on several recent works on the topic, we establish a framework using Riemann-Hilbert problems to study such polynomials. When the weight function is constant, these polynomials relate to the elliptic form of the sixth Painlevé equation. This talk is based on a recent work with Tomas Latimer and Pieter Roffelsen (arXiv: 2305.04404).

## [05496] Asymptotic prediction of tau-function zeros of Painlevé equations

**Author(s) :** Ines Varela Aniceto (University of Southampton)

**Abstract :** Transseries solutions of Painlevé I and II equations include both algebraic asymptotic expansions and exponentially small corrections, valid in pole-free regions. In this talk I will show how summing all exponential terms at each algebraic order provides an analytic continuation into the pole-filled regions of the solutions, where exponentials are no longer suppressed. The same can be done for the respective tau-functions to obtain asymptotic predictions for all the arrays of the tau-function zeros.

## [05564] Riemann-Hilbert problem on the q-Painleve equations

**Author(s) :** Yousuke Ohyama (Tokushima University)

**Abstract :** We study monodromy spaces of  $q$ -Painlevé equations. We apply the Riemann-Hilbert correspondence to analytic studies on  $q$ -Painlevé equations.

## [05591] A 3×3 Lax form for the q-P(E\_6^{(1)})

**Author(s) :** Kanam Park (Toba college)

**Abstract :** For the  $q$ -Painlevé equation with the affine Weyl group symmetry of type  $E_6^{(1)}$ , a  $2\times 2$  matrix Lax form and a second order scalar lax form were known.

In this talk, we give a  $3\times 3$  matrix Lax form and a third order scalar equation related to it. We also give its continuous limit.

These Lax form and a scalar equation seems to be new.

## [00172] On application of principle curvature distribution in local differential geometry

**Session Time & Room :** 1C (Aug.21, 13:20-15:00) @A508

**Type :** Proposal of Minisymposium

**Abstract :** Recently, shape has become increasingly crucial in device and materials science. In this symposium, we will focus on principal curvature distributions in differential geometry and discuss examples where the principal curvature distributions play a crucial role. We take particular note of the curved carbon nanotubes discovered in the 2000s, and the manufacturing methods of curved surfaces in shipbuilding and other applications. Both seem unrelated at first glance, but from an applied mathematical point of view, the principal curvature distribution is analyzed by utilizing common mathematics. This symposium aims to discuss these issues from the standpoint of local differential geometry.

**Organizer(s) :** Shigeki Matsutani, Yutaro Kabata, Yuta Ogata, Jun Onoe

**Classification :** 53A05, 53A10, 53B50

**Minisymposium Program :**

00172 (1/1) : 1C @A508 [Chair: Shigeki Matsutani]

## [04166] Fullerene and discrete principal curvature

**Format :** Talk at Waseda University

**Author(s) :** Shigeki Matsutani (Kanazawa University)Yusuke Noda (Okayama Prefectural University)

**Abstract :** Due to geometrical investigations of the carbon configurations of the first principle computations, the novel symmetry in the fullerenes, i.e., the pre-constant discrete principal curvature (pCDPC) structure, was recently found. In this talk, we show the symmetry mainly on the C<sub>60</sub> polymers and related fullerenes from geometrical viewpoints.

## [03759] Interplay between topology-induced geometry and the electronic properties of nanocarbon materials

**Format :** Talk at Waseda University

**Author(s) :** Jun Onoe (Nagoya University)

**Abstract :** The quantum mechanics in curved surface has been studied in 1950s and predicted that the electron behaviors are affected by Gaussian and average curvatures theoretically in 1980s. We have first demonstrated the quantum mechanics in submanifold experimentally using one-dimensional periodic uneven structured C<sub>60</sub> polymer formed by electron-beam irradiation of C<sub>60</sub> film.

## [04350] On discrete constant principal curvature surfaces

**Format :** Online Talk on Zoom

**Author(s) :** Yuta Ogata (Kyoto Sangyo University)

**Abstract :** In this talk, we will study the discrete surface theory on a full 3-ary oriented tree and introduce the notion of discrete principal curvatures on them. In order to investigate the geometric meaning of discrete principal curvatures, we will also define a discrete analog of curvature lines on discrete surfaces, called weak-curvature lines. At the end of the talk, we also show some examples of discrete constant principal curvature surfaces.

## [04368] Surface parametrization for manufacturing by principal curvature integral

**Format :** Online Talk on Zoom

**Author(s) :** Yutaro Kabata (Nagasaki University)

**Abstract :** The choice of coordinates is crucial in the theory of curves and surfaces. In this presentation, we discuss the appropriate way to choose coordinates for curves and surfaces from a manufacturing perspective. Specifically, we define coordinates obtained from the integration of curvature for curves and principal curvatures for surfaces, and present results related to the stratification of curves and surfaces obtained from these coordinates.

# [00176] Hyperbolic PDEs modelling non-Newtonian fluid flows

**Session Time & Room :** 5B (Aug.25, 10:40-12:20) @G605

**Type :** Proposal of Minisymposium

**Abstract :** Since the beginning of continuum mechanics, the need to improve quantitative predictions of non-Newtonian flows continues.

The simulation of turbulence or of complex (non-homogeneous) fluids using good PDEs, in particular, remains an unsatisfied goal.

A major challenge is how to conciliate the conservation principles funding physics with quantitative observations.

A natural approach is to add dissipative relaxation terms in the hyperbolic PDEs resulting of conservation laws.

The goal of the minisymposium is to confront recent advances, with promising theoretical or numerical results, regarding hyperbolic PDEs plus relaxation sources for various non-Newtonian fluid flows.

**Organizer(s) :** Sébastien Boyaval

**Classification :** 35L40, 76A05

**Minisymposium Program :**

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00176 (1/1) : 5B @G605

## [00332] Well-posedness and asymptotic behavior for hyperbolized compressible Navier-Stokes equations

**Author(s)** : Yuxi Hu (China University of Mining and Technology, Beijing)

**Abstract** : We consider the non-isentropic compressible Navier-Stokes equations (CNS) for which the heat conduction of Fourier's law is replaced by Cattaneo's law and the classical Newtonian flow is replaced by a revised Maxwell flow. We shall present our recent results on global well-posedness, finite time blow-up and asymptotic behaviour of solutions. Some qualitative behaviour of solutions are shown to be changed, i.e., Global existence VS blowup in finite time, between the classical CNS and the studied hyperbolized model, although the solutions of two system are quite close to each other for small relaxation parameter.

## [00503] Structure preserving finite element schemes for a non-Newtonian flow

**Author(s)** : Gabriel R. Barrenechea (University of Strathclyde, Glasgow, UK)Tristan Pryer (University of Bath)Emmanuil Georgoulis (Heriot-Watt University)

**Abstract** : We propose a finite element discretisation of a three-dimensional non-Newtonian flow whose dynamics are described by an Upper Convected Maxwell model. The scheme preserves structure in the sense that the velocity is divergence-free and the overall discretisation is energy consistent with the underlying problem. We investigate the problem's complexity and devise relevant timestepping strategies for efficient solution realisation. We showcase the method with several numerical experiments, confirm the theory and demonstrate the efficiency of the scheme.

## [00918] Temporal discretisation of non-Newtonian fluid flows

**Author(s)** : Ben Ashby (Heriot-Watt University, Edinburgh, UK)Tristan Pryer (University of Bath)Gabriel Barrenechea (University of Strathclyde, Glasgow)Emmanuil Georgoulis (Heriot-Watt University, UK & National Technical University of Athens, Greece)

**Abstract** : Choice of discretisation of the constitutive law for the stress in a non-Newtonian fluid is crucial for the success of any numerical method. We propose a new methodology for temporal discretisations of some non-Newtonian flows with the aim of preserving flow structure. We show that for models where both differential and integral constitutive laws are available, such as Oldroyd-B, a correspondence can be found between discretisations of both.

## [04850] New symmetric-hyperbolic PDEs for viscoelastic fluid flows

**Author(s)** : Sébastien Julien Boyaval (Ecole des Ponts ParisTech)

**Abstract** : Many Partial Differential Equations (PDEs) have been proposed to model viscoelastic flows, in between fluids and solids.

Seminal hyperbolic PDEs with stress relaxation have been proposed by Maxwell in 1867 to ensure propagation of 1D shear waves at finite-speed while capturing the viscosity of real fluid continua.

But actual computations of multi-dimensional viscoelastic flows using Maxwell's PDEs have remained limited, at least without additional diffusion that blurs the hyperbolic character of Maxwell's PDEs.

We propose a new system of PDEs to model 3D viscoelastic flows of Maxwell fluids.

Our system, quasilinear and symmetric-hyperbolic, unequivocally models smooth flows on small times, while ensuring propagation of waves at finite-speed.

Our system rigorously unifies fluid models with elastodynamics for compressible solids, and it can be extended for applications in environmental hydraulics (shallow-water flows) or materials engineering (non-isothermal flows).

# [00178] Theoretical and Computational Progress on PDE-based Inverse Problems with Applications

**Session Time & Room :**

00178 (1/3) : 2C (Aug.22, 13:20-15:00) @G808

00178 (2/3) : 2D (Aug.22, 15:30-17:10) @G808

00178 (3/3) : 2E (Aug.22, 17:40-19:20) @G808

**Type :** Proposal of Minisymposium

**Abstract :** Inverse problems for partial differential equations (PDEs) concern recovery of unknown coefficients or geometries/topologies within the equations by knowledge of certain observables. These problems sit at the intersection of mathematical analysis, PDE theory, and scientific computing, with broader application to modern imaging science and technology.

This minisymposium aims to highlight recent advances in inverse problems for PDEs. It will bring together international scientific researchers to discuss recent developments and emerging challenges in this fast-evolving field. Major topics include (1) inverse problems in wave-based imaging; (2) inverse scattering theory; (3) data-driven inverse methods, and their applications to medical and geophysical imaging.

**Organizer(s) :** Huaian Diao, Hongyu Liu, Yang Yang, Minghui Song

**Classification :** 35R30

**Minisymposium Program :**

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00178 (1/3) : 2C @G808 [Chair: Youjun Deng]

## [00556] Deterministic-Statistical Approach for Inverse Problems with Partial Data

**Format :** Online Talk on Zoom

**Author(s) :** Jiguang Sun (Michigan Technological University)

**Abstract :** We propose a deterministic-statistical approach for inverse problems with partial data. Certain deterministic method is first used to obtain useful (qualitative) information for the unknowns. Then the inverse problem is recast as a statistical inference problem and the Bayesian inversion is employed to obtain more (quantitative) information of the unknowns. Several examples are presented for demonstration. Furthermore, we introduce new statistical estimators to characterize the non-unique solutions of several inverse problems.

## [00553] Quantitative PAT with simplified PN approximation

**Format :** Online Talk on Zoom

**Author(s) :** Yimin Zhong (Auburn University)Hongkai Zhao (Duke University)

**Abstract :** The photoacoustic tomography (PAT) is a hybrid modality that combines the optics and acoustics to obtain high resolution and high contrast imaging of heterogeneous media. In this work, our objective is to study the inverse problem in the quantitative step of PAT which aims to reconstruct the optical coefficients of the governing radiative transport equation from the ultrasound measurements. In our analysis, we take the simplified P N approximation of the radiative transport equation as the physical model and then show the uniqueness and stability for this modified inverse problem. Numerical simulations based on synthetic data are presented to validate our analysis.

## [02856] Adaptive Mesh-free Approach for Gravity Inversion

**Format :** Talk at Waseda University

**Author(s) :** Yan Liu (Chinese Academy of Geological Sciences)

**Abstract :** We proposes a method of gravity inversion based on an adaptive mesh-free approach by using a modified radial basis function. As the subsurface space is generally discretized into regular grid cells, and this unstructured nodal discretization bring the expensive mesh generation and manipulation, we use a mesh-free discretization strategy to establish a mapping of subsurface grid cells to a cloud of discrete points. The nodes are adaptively refined during the inversion process to better recover abnormal bodies. In addition, the hybrid basis function and the modified radial basis function are used to improve the accuracy and stability of the solution.

## [00358] A neural network method for inverse source problem with limited-aperture data

**Format :** Talk at Waseda University

**Author(s) :** Weishi Yin (Changchun University of Science and Technology)Ping Zhang (Changchun University of Science and Technology)Pinchao Meng (Changchun University of Science and Technology)Hongyu Liu ( City University of Hong Kong)

**Abstract :** This talk is concerned with an inverse moving source problem, that is, one identifies and predicts the trajectory of a moving point source by measuring the corresponding wave field. First, for the practical consideration, the dynamical wave field data are collected in a limited aperture and full aperture respectively. Second, we design a parameter inversion model by neural network to reconstruct the trajectory of the moving point source. This model solves the problem of information loss caused by data acquisition in limited aperture and has certain robustness with respect to noise. Third, we consider the trajectory prediction of the moving point source for the inverse source problem associated with the novel input/instruction approach, and construct a trajectory prediction model by neural

network to predict the trajectory of the moving point source. Numerical experiments show that the proposed device works effectively and efficiently in some practical scenarios.

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00178 (2/3) : 2D @G808 [Chair: Hongyu Liu]

### **[00236] On plasmon modes in multi-layer structures**

**Format :** Talk at Waseda University

**Author(s) :** Youjun Deng (Central South University)

**Abstract :** We consider the plasmon resonances in multi-layer structures. We show the plasmon modes are equivalent to the eigenvalue problem of a matrix, whose order is the same to the number of layers. For any number of layers, the exact characteristic polynomial is derived by a conjecture, which is verified by using induction. It is shown that all the solutions to the characteristic polynomial are real and exist in the span [-1, 2]. Numerical examples are presented for finding all the plasmon modes.

### **[00405] Uniqueness and non-uniqueness for inverse source problems of elliptic equations**

**Format :** Talk at Waseda University

**Author(s) :** Yi-Hsuan Lin (Department of Applied Mathematics, National Yang Ming Chiao Tung University)

**Abstract :** We study inverse source problems associated to second order elliptic equations on a bounded domain. We demonstrate both uniqueness and non-uniqueness for inverse source problems of different type elliptic equations.

### **[00361] Mathematical analysis of microscale hydrodynamic cloaking and shielding using electro-osmosis**

**Format :** Talk at Waseda University

**Author(s) :** Guang-Hui Zheng (Hunan University)

**Abstract :** Rendering objects invisible by cloaking them with metamaterials have made rapid progress in the past decade. However, the difficulties of metamaterials manufacturing have limited its development. In this talk, we discuss the mathematical analysis of hydrodynamic cloaking and shielding via electro-osmosis in a microfluidic chamber that does not rely on metamaterials. Based on layer potential technique, the conditions that can ensure the occurrence of the microscale hydrodynamic cloaking and shielding are established. Finally, several numerical examples are served to validate our theoretical analysis. (joint works with Hongyu Liu (CityU) and Zhiqiang Miao (HNU))

### **[00920] Regularizing Effect of Damping Mechanisms in Inverse Problems of Evolution Equations**

**Format :** Talk at Waseda University

**Author(s) :** Sakthivel Kumarasamy (Indian Institute of Space Science and Technology )Alemdar Hasanov Hasanoglu (Kocaeli University, Turkey)Anjuna Dileep (Indian Institute of Space Science and Technology )

**Abstract :** It is known that the undamped evolution models, such as the Euler-Bernoulli beam, and Kirchhoff-Love plate, don't support the unique determination of unknown spatial load from the measured displacement at the final time. We solve this issue by introducing the viscous external damping and Kelvin-Voigt damping effects in the basic governing equations. The damping terms play a pivotal role in getting more regular solutions with less regular data on the direct problem, while in the context of inverse problems, it has a similar effect to a regularization term in the Tikhonov functional of the quasi-solution approach.

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00178 (3/3) : 2E @G808 [Chair: Yang Yang]

### **[00359] A NOVEL QUANTITATIVE INVERSE SCATTERING SCHEME USING INTERIOR RESONANT MODES**

**Format :** Talk at Waseda University

**Author(s) :** Xianchao Wang (Harbin Institute of Technology)

**Abstract :** In this talk, we introduce a novel quantitative imaging scheme to identify impenetrable obstacles in time-harmonic acoustic scattering from the associated far-field data. The proposed method consists of two phases. In the first phase, we determine the interior eigenvalues of the underlying unknown obstacle from the far-field data via the indicating behaviour of the linear sampling method. Then we further determine the associated interior eigenfunctions by solving a constrained optimization problem, again only involving the far-field data. In the second phase, we propose a novel iteration scheme of Newton's type to identify the boundary surface of the obstacle. By using the interior eigenfunctions determined in the first phase, we can avoid computing any direct scattering problem at each Newton's

iteration. The proposed method is particularly valuable for recovering a sound-hard obstacle, where the Newton's formula involves the geometric quantities of the unknown boundary surface in a natural way.

### [00333] Simultaneous recovery of a scattering cavity and its internal sources

**Format :** Talk at Waseda University

**Author(s) :** Deyue Zhang (Jilin University) Yukun Guo (Harbin Institute of Technology) Yinglin Wang (Jilin University) Yan Chang (Harbin Institute of Technology)

**Abstract :** We consider the simultaneous reconstruction of a sound-soft cavity and its excitation sources from the total-field data. Using the single-layer potential representations on two measurement curves, this problem can be decoupled into an inverse cavity scattering problem and an inverse source problem. Then the uncoupled subproblems are respectively solved by the modified optimization and sampling method. Numerical examples will be presented to demonstrate the effectiveness of the method.

### [00259] The anisotropic Calderón problem at large fixed frequency on manifolds with invertible ray transform

**Format :** Talk at Waseda University

**Author(s) :** Shiqi Ma (Jilin University)

**Abstract :** We consider the inverse problem of recovering a potential from the Dirichlet to Neumann map at a large fixed frequency on certain Riemannian manifolds. We extend the earlier result of [ G. Uhlmann and Y. Wang, arXiv:2104.03477] to the case of simple manifolds, and more generally to manifolds where the geodesic ray transform is stably invertible.

### [00245] Minnaert resonances for bubbles in soft elastic materials

**Format :** Online Talk on Zoom

**Author(s) :** Hongjie LI (The Chinese University of Hong Kong)

**Abstract :** In this talk, the low-frequency resonance for acoustic bubbles embedded in soft elastic materials is discussed. This is a hybrid physical process that couples the acoustic and elastic wave propagations. By delicately and subtly balancing the acoustic and elastic parameters as well as the geometry of the bubble, we show that Minnaert resonance can occur for rather general constructions. This study poses a great potential for the effective realisation of negative elastic materials by using bubbly elastic media.

## [00179] Advances in forward and inverse problems of wave equations

**Session Time & Room :**

00179 (1/3) : 3C (Aug.23, 13:20-15:00) @E709

00179 (2/3) : 3D (Aug.23, 15:30-17:10) @E709

00179 (3/3) : 3E (Aug.23, 17:40-19:20) @E709

**Type :** Proposal of Minisymposium

**Abstract :** The recent advances in wave equations and its fast numerical methods have provided useful tools for many applications ranging from nano-optics to medical imaging and geosciences. This mini-symposium will discuss the challenges in the formulations of forward and inverse problems, cutting edge fast algorithms and their efficient implementation and applications in various fields. At the same time, it will provide opportunities to promote interdisciplinary research collaboration between computational scientists and other fields.

**Organizer(s) :** Carlos Borges, Jun Lai

**Classification :** 65N21, 45Q05, 31A10, 31B10, 78M99

**Minisymposium Program :**

00179 (1/3) : 3C @E709 [Chair: Jun Lai]

## [00347] Accurate evaluation of Helmholtz layer potentials using Quadrature by two expansions

**Format :** Talk at Waseda University

**Author(s) :** Min Hyung Cho (University of Massachusetts Lowell)Jared Weed (University of Massachusetts Lowell)Lingyun Ding (University of California Los Angeles)Jingfang Huang (University of North Carolina at Chapel Hill)

**Abstract :** The Helmholtz layer potentials are evaluated using the Quadrature by two expansions (QB2X). The QB2X method uses local complex Taylor expansion and planewave-type expansions to achieve a representation that is numerically accurate at all target points inside the leaf box in the hierarchical tree structure. Compared with the original quadrature by the expansion that uses only the local expansion, the QB2X includes explicit nonlinearity from the boundary geometry in the planewave type expansions and it follows standard fast multipole method error analysis. Therefore, QB2X overcomes many challenges quadrature by expansion has and is suitable for complex geometry. The main ideas of the derivation of QB2X using Fourier extension and contour integrals, and numerical results showing the efficiency of QB2X compared with the quadrature by expansion will be presented for both flat and curved boundaries.

## [00411] On the Robustness of Inverse Scattering for Penetrable, Homogeneous Objects

**Format :** Talk at Waseda University

**Author(s) :** Borges Carlos (University of Central Florida)Manas Rachh (Flatiron Institute)Leslie Greengard (New York University and Flatiron Institute)

**Abstract :** In the inverse obstacle scattering problem, one determines the shape of a domain from measurements of the scattered field due to a set of incident fields. For a penetrable obstacle with known sound speed, this can be accomplished by treating the boundary alone as an unknown curve. Alternatively, one can treat the entire object as an unknown and use a volumetric representation, without making use of the known sound speed. Both lead to strongly nonlinear and nonconvex optimization problems for which recursive linearization provides a useful framework. After extending our shape optimization approach developed earlier for impenetrable bodies to penetrable obstacles, we carry out a systematic study of both methods and compare their performance on a variety of examples. Our findings indicate that the volumetric approach is more robust, even though the number of degrees of freedom is significantly larger.

## [00490] A Neural Network Warm-Start Approach for the Inverse Acoustic Obstacle Scattering Problem

**Format :** Talk at Waseda University

**Author(s) :** Manas Rachh (Flatiron Institute)Mo Zhou (Duke University)Jiequn Han (Flatiron Institute)Borges Carlos (University of Central Florida)

**Abstract :** We consider the inverse acoustic obstacle problem for sound-soft star-shaped obstacles in two dimensions. The inverse problem is computationally challenging since the local set of convexity shrinks with increasing frequency and results in an increasing number of local minima in the vicinity of the true solution. In this talk, we present a neural network warm-start approach for solving the inverse scattering problem, where an initial guess is obtained using a trained neural network.

## [04073] Optimal Transportation for Electrical Impedance Tomography

**Format :** Talk at Waseda University

**Author(s) :** Gang BAO (Zhejiang University)Yixuan Zhang (Zhejiang University)

**Abstract :** A new framework is introduced for solving inverse boundary problems with the geodesic based quadratic Wasserstein distance. A general form of the Fréchet gradient is systematically derived by optimal transportation (OT) theory. A fast algorithm based on the new formulation of OT is developed to solve the corresponding optimal transport problem with much improved computational complexity. This framework provides a new computational approach for solving the challenging electrical impedance tomography problem.

00179 (2/3) : 3D @E709 [Chair: Carlos Borges]

## [03446] A high-accuracy boundary integral equation method for wave scattering by 3D analytic surfaces

**Format :** Talk at Waseda University

**Author(s) :** Wangtao Lu (Zhejiang University)Jun Lai (Zhejiang University)

**Abstract :** In this talk, we present a high accuracy boundary integral equation method for wave scattering by a closed analytic surface. The surface is assumed to parameterize in earth-like latitude and longitude coordinates. Any analytic function on it can be firstly approximated by its Fourier series in the latitude variable, and then piecewise Legendre

part\_1

polynomials in the longitude variable. By doing so, we can accurately approximate the standard single-, double-, and adjoint double-layer integral operators in two stages. First, the integrals in the latitude direction are approximated by a nearly optimal algorithm for computing the Fourier transforms of the related kernel functions. Second, the resulting single-variable integrals in the latitude direction have weakly singular kernels, and can be spectrally discretized by pre-designed high-accuracy quadrature rules. We study exterior and interior boundary value problems to validate efficiency and accuracy of the proposed method.

## [03520] Fast algorithms for multiple elastic obstacles scattering and inverse scattering

**Format :** Talk at Waseda University

**Author(s) :** Jun Lai (Zhejiang University)

**Abstract :** Elastic wave scattering and inverse scattering have been appeared in a lot of important applications, including non-destructive testing, seismic inversion, and medical imaging, etc. Integral equation method provides an effective tool for solving elastic wave scattering and inverse scattering problems. In this talk, fast and high order numerical methods based on integral equations will be presented for elastic wave equations in the presence of multiple obstacles. In particular, I will talk about the numerical algorithms using high order discretization of singular integrals and the fast multipole method for evaluating the multiple elastic scattering problem, as well as their applications in the inverse elastic wave scattering based on the time reversal method.

## [05069] Exploring inverse obstacle scattering with an impedance model

**Format :** Talk at Waseda University

**Author(s) :** Travis Askham (New Jersey Institute of Technology)Manas Rachh (Flatiron Institute)Carlos Borges (University of Central Florida)Jeremy Hoskins (University of Chicago)

**Abstract :** It is well known that in certain limits the impedance boundary condition can mimic the sound hard, sound soft, and transmission boundary conditions. Here we explore the performance of this approximation in inverse obstacle scattering problems. We find that for certain problems a relaxation of the usual measurement of scattering error improves the quality of obstacle recovery.

## [03858] Hybrid methods for the application of singular integral operators

**Format :** Talk at Waseda University

**Author(s) :** Leslie Greengard (New York University and Flatiron Institute)Shidong Jiang (Flatiron Institute)Jun Wang (Tsinghua University)Fredrik Fryklund (Courant Institute, NYU)Samuel F Potter (Courant Institute, NYU)

**Abstract :** We present hybrid asymptotic/numerical methods for the accurate computation of elliptic and parabolic volume and layer potentials in two and three dimensions.

00179 (3/3) : 3E @E709 [Chair: Carlos Borges]

## [04029] Obstacles and interfaces composite scattering in a multilayered medium

**Format :** Talk at Waseda University

**Author(s) :** Lei Zhang (Zhejiang University of Technology)

**Abstract :** This talk will focus on the mathematical analysis and numerical methods for the composite scattering problem from obstacles and interfaces in a multilayered medium. We will highlight some recent progress in this area. Specifically, we will address how to handle obstacles and rough surfaces, and how to model scattering from unbounded surfaces. We will also discuss the well-posedness and numerical methods for solving these problems based on the characteristic of the scattering problems.

## [04887] Lippmann Schwinger integral equation for fiber optics analysis

**Format :** Talk at Waseda University

**Author(s) :** Felipe Vico (UPV)Miguel Ferrando-Bataller (UPV)Eva Antonino-Daviu (UPV)Marta Cabedo-Fabrés (UPV)

**Abstract :** In this talk, we will present a Lippmann-Schwinger integral formulation for accurately calculating the propagating modes in fiber optics. Our formulation is based on a second-kind integral equation, which ensures stability in the presence of noise and uncertainties. Furthermore, our discretization scheme exhibits superalgebraic convergence for smooth refractive index fibers, making it suitable for graded-index fibers.

## [05178] Single-excitation quantum optics: analysis and algorithms

**Format :** Talk at Waseda University

**Author(s) :** Jeremy Graeme Hoskins (University of Chicago)Jeremy Hoskins (University of Chicago)Manas Rachh (Flatiron Institute)John Schotland (Yale University)Jason Kaye (Flatiron Institute, Simons Foundation)

**Abstract :** Recent progress in experimental quantum optics has facilitated the physical construction of systems of increasing complexity. Of particular importance are experiments involving the scattering of one or two photons from a collection of atoms. In this context, a central question is to understand the time evolution of the entanglement between atoms, mediated by the field. In this talk we will discuss analytical results on the properties of these systems, and how those properties depend on disorder or distribution of the locations of the atoms.

## [05639] Poisson Solver for Complicated Geometries in R3 Using Function Extension

**Author(s) :** Fredrik Fryklund (New York University)Charles Epstein (Flatiron Institute, Simons Foundation)Shidong Jiang (Flatiron Institute, Simons Foundation)Leslie Greengard (Flatiron Institute, Simons Foundation)

**Abstract :** We describe a new, adaptive solver for the three-dimensional Poisson equation in complicated geometries. The solution is represented as the sum of a volume potential and a double layer potential. The source data is extended with high order accuracy along the normals to the surface, to a geometrically simpler region. This allows us to accelerate the evaluation of the volume potential using an FMM.

## [00184] Recent advances in data-driven methods for inverse problems

**Session Time & Room :**

00184 (1/4) : 4C (Aug.24, 13:20-15:00) @E811

00184 (2/4) : 4D (Aug.24, 15:30-17:10) @E811

00184 (3/4) : 4E (Aug.24, 17:40-19:20) @E811

00184 (4/4) : 5B (Aug.25, 10:40-12:20) @E811

**Type :** Proposal of Minisymposium

**Abstract :** The remarkable success of deep learning has led to a transformative impact on the research landscape of inverse problems in imaging. This mini-symposium aims to bring together researchers who have made exciting contributions to understanding the theoretical foundations and empirical performance of deep learning in various imaging applications. The talks will cover a wide range of topics such as deep regularization, Bayesian methods, microlocal analysis, learned optimization solvers, and robustness of reconstruction methods to distribution shift and adversarial attacks, making the sessions of sufficient interest to a broad audience, while encouraging an exchange of ideas to advance the state-of-the-art.

**Organizer(s) :** Subhadip Mukherjee, Carola-Bibiane Schönlieb, Martin Burger

**Classification :** 68T07, 65J22, deep learning, inverse problems in imaging

**Minisymposium Program :**

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00184 (1/4) : 4C @E811

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00184 (2/4) : 4D @E811 [Chair: Carola-Bibiane Schönlieb]

## [05418] Machine learned regularization for inverse problems - the dos and don'ts

**Format :** Online Talk on Zoom

**Author(s) :** Carola-Bibiane Schönlieb (University of Cambridge)

**Abstract :** Inverse problems are about the reconstruction of an unknown physical quantity from indirect measurements. They appear in a variety of places, from medical imaging, for instance MRI or CT, to remote sensing, for instance Radar, to material sciences and molecular biology, for instance electron microscopy. Here, inverse problems is a tool for looking inside specimen, resolving structures beyond the scale visible to the naked eye, and to quantify them. It is a mean for diagnosis, prediction and discovery.

Most inverse problems of interest are ill-posed and require appropriate mathematical treatment for recovering

meaningful solutions. Classically, such approaches are derived almost conclusively in a knowledge driven manner, constituting handcrafted mathematical models. Examples include variational regularization methods with Tikhonov regularization, the total variation and several sparsity-promoting regularizers such as the L1 norm of Wavelet coefficients of the solution. While such handcrafted approaches deliver mathematically rigorous and computationally robust solutions to inverse problems, they are also limited by our ability to model solution properties accurately and to realise these approaches in a computationally efficient manner.

Recently, a new paradigm has been introduced to the regularization of inverse problems, which derives solutions to inverse problems in a data driven way. Here, the inversion approach is not mathematically modelled in the classical sense, but modelled by highly over-parametrised models, typically deep neural networks, that are adapted to the inverse problems at hand by appropriately selected training data. Current approaches that follow this new paradigm distinguish themselves through solution accuracies paired with computational efficiency that were previously unconceivable.

In this talk I will give an introduction to this new data-driven paradigm for inverse problems. Presented methods include data-driven variational models and plug-and-play approaches, learned iterative schemes aka learned unrolling, and learned post-processing. Throughout presenting these methodologies, we will discuss their theoretical properties and provide numerical examples for image denoising, deconvolution and computed tomography reconstruction. The talk will finish with a discussion of open problems and future perspectives.

## **[04644] Data-driven Regularization based on Diagonal Frame Decompostion**

**Format :** Talk at Waseda University

**Author(s) :** Yunseok Lee (Ludwig Maximilian University Munich)Samira Kabri (Deutsches Elektronen-Synchrotron (DESY) Hamburg)Martin Burger (Deutsches Elektronen-Synchrotron (DESY) Hamburg and University of Hamburg)Gitta Kutyniok (Ludwig Maximilian University Munich)

**Abstract :** In this talk, we propose a data-driven framework to design optimal filters for inverse problems using frame decompositions, which generalize classical spectral filters. Frames are sets of vectors that allow for stable and redundant representations of signals in a Hilbert space. Our framework works by learning a linear transformation that modifies the frame coefficients of a measured signal to enhance or suppress certain features. This is achieved by formulating this as an optimization problem with a data-driven regularizer that incorporates prior knowledge from noise and ground truth data. Our approach comes with theoretical guarantees in terms of convergence as well as in terms of generalization to unseen data. We also illustrate its effectiveness on several numerical experiments using the Wavelet-Vaguelette decomposition as an example.

## **[03944] Fourier Neural Operators for data-driven regularization**

**Format :** Talk at Waseda University

**Author(s) :** Samira Kabri (Friedrich-Alexander-Universität Erlangen-Nürnberg)

**Abstract :** In this talk we investigate the use of Fourier Neural Operators (FNOs) for image processing in comparison to standard Convolutional Neural Networks (CNNs). FNOs - which are so-called neural operators with a specific parametrization - have been applied successfully in the context of parametric PDEs. We derive the FNO architecture as an example for continuous and Fréchet-differentiable neural operators on Lebesgue spaces and show how CNNs can be converted into FNOs and vice versa. Based on these insights, we explore possibilities of incorporating the ideas of FNOs into the data-driven regularization of inverse problems in imaging.

## **[05027] Data-driven regularization theory of invertible ResNets for solving inverse problems**

**Format :** Online Talk on Zoom

**Author(s) :** Clemens Arndt (ZeTeM University of Bremen)Alexander Denker (ZeTeM University of Bremen)Sören Dittmer (ZeTeM University of Bremen)Nick Heilenkötter (ZeTeM University of Bremen)Meira Iske (ZeTeM University of Bremen)Tobias Kluth (University of Bremen)Judith Nickel (ZeTeM University of Bremen)

**Abstract :** Data-driven solution techniques for inverse problems, typically based on specific learning strategies, exhibit remarkable performance in image reconstruction tasks. These learning-based reconstruction strategies often follow a two-step scheme. First, one uses a given dataset to train the reconstruction scheme, which one often parametrizes via a neural network. Second, the reconstruction scheme is applied to a new measurement to obtain a reconstruction. We follow these steps but specifically parametrize the reconstruction scheme with invertible residual networks (iResNets). We demonstrate that the invertibility opens the door to new investigations into the influence of the training and the architecture on the resulting reconstruction scheme. To be more precise, we analyze the effect of different iResNet architectures, loss functions, and prior distributions on the trained network. The investigations reveal a formal link to the regularization theory of linear inverse problems for shallow network architectures. Moreover, we analytically optimize the parameters of specific classes of architectures in the context of Bayesian inversion, revealing the influence of the prior and noise distribution on the solution.

## [05430] Are neural operators really neural operators?

**Format :** Online Talk on Zoom

**Author(s) :** Rima Alaifari (ETH Zurich)

**Abstract :** In operator learning, it has been observed that proposed models may not behave as operators when implemented, questioning the very essence of what operator learning should be. We contend that some form of continuous-discrete equivalence is necessary for an architecture to genuinely learn the underlying operator, rather than just discretizations of it. Employing frames, we introduce the framework of Representation equivalent Neural Operator (ReNO) to ensure operations at the continuous and discrete level are equivalent.

## [04722] Plug-and-Play Models for Large-Scale Computational Imaging

**Format :** Talk at Waseda University

**Author(s) :** Ulugbek Kamilov (Washington University in St. Louis)

**Abstract :** Computational imaging is a rapidly growing area that seeks to enhance the capabilities of imaging instruments by viewing imaging as an inverse problem. Plug-and-Play Priors (PnP) is one of the most popular frameworks for solving computational imaging problems through integration of physical and learned models. PnP leverages high-fidelity physical sensor models and powerful machine learning methods to provide state-of-the-art imaging algorithms. PnP models alternate between minimizing a data-fidelity term to promote data consistency and imposing a learned image prior in the form of an “image denoising” deep neural network. This talk presents a principled discussion of PnP, its theoretical foundations, its implementations for large-scale imaging problems, and recent results on PnP for the recovery of continuously represented images. We present several applications of our theoretical and algorithmic insights in bio-microscopy, computerized tomography, and magnetic resonance imaging.

## [02097] Learned proximal operators meets unrolling for limited angle tomography

**Format :** Online Talk on Zoom

**Author(s) :** Tatiana Alessandra Bubba (University of Bath)Subhadip Mukherjee (University of Bath)Luca Ratti (University of Genoa)Andrea Sebastiani (University of Bologna)

**Abstract :** In recent years, limited angle tomography has become a challenging testing ground for several theoretical and numerical studies, where both variational regularisation and data-driven techniques have been investigated extensively. I will present a hybrid reconstruction framework where the proximal operator of an accelerated unrolled scheme is learned to ensure suitable theoretical guarantees. The recipe relays on the interplay between sparse regularisation, harmonic analysis, microlocal analysis and Plug and Play methods.

## [04626] Plug-and-Play sampling for inverse problems in imaging

**Format :** Talk at Waseda University

**Author(s) :** Julie Delon (Université Paris Cité)Rémi Laumont (Technical University of Denmark,)Marcelo Pereyra (Heriot-Watt University)Andrés Almansa (Université Paris Cité)Valentin De Bortoli (Ecole Normale Supérieure)

**Abstract :** In a Bayesian framework, image models are used as priors or regularisers and combined to explicit likelihood functions to define posterior distributions. These posterior distributions can be used to derive Maximum A Posteriori (MAP) estimators, leading to optimization problems that are generally well studied and understood. Sampling schemes can also be used to explore more finely these posterior distributions, derive other estimators, quantify uncertainties or perform other advanced inferences. In a manner akin to Plug & Play (PnP) methods in optimization, these sampling schemes can be combined with denoising neural networks approximating the gradient of a log-prior on images. In this talk, we will focus on these PnP sampling schemes, which raise important questions concerning the correct definition of the underlying Bayesian models or the computed estimators, as well as their regularity properties, necessary to ensure the stability of the numerical schemes.

00184 (4/4) : 5B @E811 [Chair: Subhadip Mukherjee]

## [03828] Recent advance of diffusion models in inverse problems

**Format :** Talk at Waseda University

**Author(s) :** Jong Chul YE (KAIST)

**Abstract :** Recently, diffusion models have been used to solve various inverse problems for medical imaging applications in an unsupervised manner. In this talk, we propose an additional correction term inspired by the manifold constraint, which can be used synergistically with the previous solvers to make the iterations close to the manifold.

## [04409] Conditional Image Generation with Score Based Models

**Format :** Talk at Waseda University

**Author(s) :** Jan Paweł Stanczuk (University of Cambridge)Georgios Batzolis (University of Cambridge)

**Abstract :** Score-based diffusion models have emerged as one of the most promising frameworks for deep generative modelling. In this work we conduct a systematic comparison and theoretical analysis of different approaches to learning conditional probability distributions with score-based diffusion models. In particular, we prove results which provide a theoretical justification for one of the most successful estimators of the conditional score. Moreover, we introduce a multi-speed diffusion framework, which leads to a new estimator for the conditional score, performing on par with previous state-of-the-art approaches.

## [01555] Data-Driven Convex Optimization via Mirror Descent

**Format :** Talk at Waseda University

**Author(s) :** Hong Ye Tan (University of Cambridge)Subhadip Mukherjee (University of Bath)Junqi Tang (University of Cambridge)Carola Bibiane Schoenlieb (University of Cambridge)Andreas Hauptmann (University of Oulu)

**Abstract :** Learning-to-optimize is an emerging framework that seeks to speed up the solution of certain optimization problems by leveraging training data. We propose a provably approximately convergent learning-to-optimize scheme for convex optimization based on a functional parameterization of the classical mirror descent algorithm. In particular, we model the underlying convex function with an input-convex neural network and derive corresponding convergence rate bounds. We demonstrate improved convergence rates on various convex image processing examples.

## [03784] Multi-Modal Hypergraph Diffusion Network with Dual Prior for Alzheimer Classification

**Format :** Talk at Waseda University

**Author(s) :** Angelica Aviles-Rivero (University of Cambridge)

**Abstract :** The automatic early diagnosis of prodromal stages of Alzheimer's disease is of great relevance for patient treatment to improve quality of life. We address this problem as a multi-modal classification task. Multi-modal data provides richer and complementary information. However, existing techniques only consider lower order relations between the data and single/multi-modal imaging data. In this work, we introduce a novel semi-supervised hypergraph learning framework for Alzheimer's disease diagnosis. Our framework allows for higher-order relations among multi-modal imaging and non-imaging data whilst requiring a tiny labelled set. Firstly, we introduce a dual embedding strategy for constructing a robust hypergraph that preserves the data semantics. We achieve this by enforcing perturbation invariance at the image and graph levels using a contrastive based mechanism. Secondly, we present a dynamically adjusted hypergraph diffusion model, via a semi-explicit flow, to improve the predictive uncertainty.

# [00185] AAA rational approximation: extensions and applications

**Session Time & Room :**

00185 (1/2) : 4C (Aug.24, 13:20-15:00) @F310

00185 (2/2) : 4D (Aug.24, 15:30-17:10) @F310

**Type :** Proposal of Minisymposium

**Abstract :** The numerical computation of rational approximations has become much easier since the appearance of the AAA algorithm in 2018. This minisymposium will explore some of the many things that have happened since then.

**Organizer(s) :** Lloyd N. Trefethen

**Classification :** 41A20, 65D15

**Minisymposium Program :**

00185 (1/2) : 4C @F310 [Chair: Nick Trefethen]

## [02196] Review of AAA approximation

**Format :** Talk at Waseda University

**Author(s) :** Lloyd Nicholas Trefethen (University of Oxford)

**Abstract :** The AAA ("triple A") algorithm is a fast and reliable black box algorithm for computing rational approximations to real or complex functions. It has been used by many people since its publication in 2018. This talk will be an introduction to AAA and its applications.

## [05528] pAAA for multivariate functions and AAA-LQO for systems with quadratic outputs

**Format :** Online Talk on Zoom

**Author(s) :** Serkan Gugercin (Virginia Tech)

**Abstract :** We first introduce the parametric-AAA (pAAA) algorithm for approximating multivariate functions, such as the transfer functions of parametric dynamical systems, where the approximant is constructed in the multivariate barycentric form. We then develop the barycentric form for linear dynamical systems with quadratic outputs (LQO). This new formulation leads to the AAA-LQO algorithm.

## [02708] Rational approximation for noisy data

**Format :** Talk at Waseda University

**Author(s) :** Anil Damle (Cornell University)

**Abstract :** Approximation of data by rational functions has many clear upsides over other representational forms. However, even if a rational function provides an effective underlying model for a given task the data it must be built from is often corrupted by noise. In this talk we will explore how existing rational approximation algorithms are impacted by noise, and discuss algorithms that are specifically tailored to effectively and efficiently build rational approximations of noisy data.

## [03138] SO-AAA: learning systems with second-order dynamics

**Format :** Talk at Waseda University

**Author(s) :** Ion Victor Gosea (Max Planck Institute for Dynamics of Complex Technical Systems)Serkan Gugercin (Virginia Tech University)Steffen W. R. Werner (New York University)

**Abstract :** The AAA (Adaptive Antoulas Anderson) algorithm is a rational approximation tool used to fit rational functions to data measurements. We present here an extension of AAA to fitting systems with second-order dynamics (structured case). Toward this goal, the development of structured barycentric forms associated with the transfer function of second-order systems is needed. These allow the iterative construction of reduced-order models from given frequency domain data, by combining interpolation and least-squares fit.

00185 (2/2) : 4D @F310 [Chair: Nick Trefethen]

## [02698] Linearization of dynamical systems using the AAA algorithm

**Format :** Talk at Waseda University

**Author(s) :** Karl Meerbergen (KU Leuven)

**Abstract :** We provide an overview of the use of AAA for the linearization of all kinds of nonlinear equations arising from dynamical systems. This includes nonlinear eigenvalue problems, nonlinear frequency dependent dynamical systems and nonlinear time dependent systems. The concept linearization is key for these problems, since linear problems are usually easier to handle in numerics.

## [02371] Time-domain model reduction in the Loewner framework

**Format :** Talk at Waseda University

**Author(s) :** Athanasis Antoulas (Rice University)

**Abstract :** In this talk we will present the main features of the Loewner Framework for rational approximation and model reduction. In particular, time domain methods will be of central importance.

## [05435] AAA and numerical conformal mapping

**Format :** Online Talk on Zoom

**Author(s) :** Olivier Sète (University of Greifswald)

**Abstract :** In this talk, we explore applications of AAA rational approximation in numerical conformal mapping.

**[05536] AAA rational approximation on a continuum****Format** : Talk at Waseda University**Author(s)** : Yuji Nakatsukasa (University of Oxford)**Abstract** : AAA has normally been applied on a discrete set, typically hundreds or thousands of points in a (real or complex) domain. Here we introduce a continuum AAA algorithm that discretizes a domain adaptively as it goes, which often also reduces the number of samples required. The key idea is that the support points tend to indicate where more samples are required. Execution is fast since SVDs are computed only for matrices that are nearly square.**[00187] Analysis and geometry of inextensible materials****Session Time & Room** : 3C (Aug.23, 13:20-15:00) @G801**Type** : Proposal of Minisymposium**Abstract** : There are many objects in the world around us that can be modeled as inextensible: pipes, chains, ribbons, cloth, whips, flagella, filaments, macromolecules, soft robot links, yarn, flags, cables in the ocean, galactic motion and octopus tentacles. In a certain sense, the inextensibility interpolates between rigid bodies and incompressible fluids but in comparison to them has many genuinely new difficulties due to the presence of unknown Lagrange multipliers. We intend to bring together some of the leading experts to discuss the modern ways to handle the analytical complexity of the PDE related to inextensible materials and the beautiful underlying geometry.**Organizer(s)** : Dmitry Vorotnikov**Classification** : 35Qxx, 58Exx, 74Hxx**Minisymposium Program** :

00187 (1/1) : 3C @G801 [Chair: Dmitry Vorotnikov]

**[02002] Modeling and Simulation of Thin Sheet Folding****Format** : Talk at Waseda University**Author(s)** : Soeren Bartels (University of Freiburg)**Abstract** : The folding of a thin elastic sheet along a curved arc has various applications including the construction of bistable devices. We discuss the derivation of a plate model from three-dimensional hyperelasticity and rigidity properties of admissible deformations and minimizers. The numerical solution is based on an isoparametric discontinuous Galerkin finite element method that provides a suitable geometric approximation of the folding arc. Error estimates are presented for a linearized version of the model problem.**[02066] Periodic partitions with minimal perimeter****Format** : Talk at Waseda University**Author(s)** : Matteo Novaga (University of Pisa)Annalisa Cesaroni (University of Padova)**Abstract** : I will discuss existence and regularity of fundamental domains which minimize a general perimeter functional in a homogeneous metric measure space. In the planar case I will give a detailed description of the domains which are minimal for a general anisotropic perimeter.**[02439] Inextensible elastic curves and subriemannian manifolds****Format** : Talk at Waseda University**Author(s)** : Chun-Chi Lin (National Taiwan Normal University)National Taiwan Normal University)**Abstract** : Elastic curves are relatively simple geometric objects in differential geometry but are related to many applications in image sciences and geometric control theory.

These curves are characterized by the equilibrium configurations of the energy functional,

$$\int (a + b \cdot |\vec{\kappa}|^2) ds,$$

where  $a, b$  are positive constants,  $\vec{\kappa}$  is the curvature vector of curves and  $s$  is the arclength of curves.

The Euler-Lagrange equations are fourth-order differential equations of the curves.

On the other hand, an energy decreasing flow of inextensible elastic curves in the plane can be formulated by a second-order parabolic equation with Lagrange multipliers.

However, difficulties come out as one generalizes this approach to curves in higher dimensional Euclidean spaces or Riemannian manifolds.

In this talk, we are interested in relating inextensible elastic curves to geometric analysis of curves in subriemannian

manifolds.

We will introduce a different approach for problem and demonstrate our progress and results.

## [02016] Gradient flows of inextensible networks

**Format :** Talk at Waseda University

**Author(s) :** Dmitry Vorotnikov (Universidade de Coimbra )

**Abstract :** We address solvability of equations of overdamped motion of inextensible networks. Problems of this kind can be expressed as PDE that involve unknown Lagrange multipliers and non-standard boundary conditions related to the moving junctions. They can also be interpreted as gradient flows on certain "manifolds" of probability measures. We also discuss the geometry of these manifolds as well as links of our equations to the mean curvature flow and to fluid dynamics.

## [00193] Adversarial robustness at the interface of analysis, geometry and statistics

**Session Time & Room :**

00193 (1/3) : 5B (Aug.25, 10:40-12:20) @E503

00193 (2/3) : 5C (Aug.25, 13:20-15:00) @E503

00193 (3/3) : 5D (Aug.25, 15:30-17:10) @E503

**Type :** Proposal of Minisymposium

**Abstract :** Stability and robustness have emerged as essential properties for modern machine learning methods. In this three-part minisymposium, we gather researchers from mathematics, statistics, and computer science that have been driving the research in this field in a variety of directions, offering a platform for scientific exchange and aiming at sparking new collaborations in this vibrant and important field.

Some of the topics that will be covered by this mini-symposium include regularization methods and insights from variational calculus for training robust models, numerical methods for solving min-max problems, distributionally robust optimization, GANs, geometric insights on adversarial robustness, among others.

**Organizer(s) :** Tim Roith, Nicolás García Trillos, Martin Burger

**Classification :** 62Gxx, 68Q32, 49Qxx

**Minisymposium Program :**

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00193 (1/3) : 5B @E503 [Chair: Nicolás García Trillos]

## [00265] Distributionally Robust Gaussian Process Regression and Bayesian Inverse Problems

**Format :** Talk at Waseda University

**Author(s) :** Jose Blanchet (Stanford)

**Abstract :** We study a distributionally robust optimization formulation (i.e., a min-max game) for two representative problems in Bayesian nonparametric estimation: Gaussian process regression and, more generally, linear inverse problems. Our formulation seeks the best mean-squared error predictor, in an infinite-dimensional space, against an adversary who chooses the worst-case model in a Wasserstein ball around a nominal infinite-dimensional Bayesian model. The transport cost is chosen to control features such as the degree of roughness of the sample paths that the adversary is allowed to inject. We show that the game has a well-defined value (i.e., strong duality holds in the sense that max-min equals min-max) and that there exists a unique Nash equilibrium which can be computed by a sequence of finite-dimensional approximations. Crucially, the worst-case distribution is itself Gaussian. We explore properties of the Nash equilibrium and the effects of hyperparameters through a set of numerical experiments, demonstrating the versatility of our modeling framework.

## [01932] Adversarial distributional robustness from Wasserstein ascent-descent particle dynamics

**Format :** Talk at Waseda University

**Author(s) :** Camilo García Trillos (University College London)Nicolas Garcia Trillos (University of Wisconsin Madison)

**Abstract :** We propose iterative algorithms to solve adversarial problems in a variety of supervised learning settings. Our algorithms, suggested by ascent-descent dynamics in a projected Wasserstein space, take the form of a system of

part\_1

interacting particles. We show the particle dynamics converge toward mean-field limit equations as the number of particles grows. In turn, the mean-field dynamics converge, as time goes to infinity, to epsilon-Nash equilibria of the original adversarial learning problem. We study, moreover, some advantages found on a nonconvex- strongly concave case -in a sense to be made precise in the talk-. Joint work with Nicolás García Trillo.

## [00273] Optimal Algorithms for Stochastic Nested Composition Optimization with Applications to Robust Training

**Format :** Talk at Waseda University

**Author(s) :** Krishnakumar Balasubramanian (UC Davis)

**Abstract :** Many robust training problems could be cast in the form of optimizing a nested composition of  $T$  functions. Examples include distributionally robust optimization, risk-averse learning, robust meta learning, etc. In this talk, I will discuss stochastic optimization algorithms for minimizing nested composition of  $T$  functions with and without bi-level structures. Assuming access to noisy evaluations of the functions and their gradients through a stochastic first-order oracle, I will present an algorithm using moving-average stochastic estimates for solving the above problem. We show that the proposed algorithm can achieve a sample complexity of  $\mathcal{O}(1/\epsilon^4)$  for converging to an  $\epsilon$ -stationary point of the problem. To the best of our knowledge, this is the first time that such an online algorithm designed for the (un)constrained multi-level setting, obtains the optimal sample complexity of the smooth single-level setting, under mild assumptions on the stochastic first-order oracle.

## [00274] Convergence of GDA for mean field two-player zero-sum games

**Format :** Talk at Waseda University

**Author(s) :** Yulong Lu (University of Massachusetts Amherst)

**Abstract :** Min-max optimization problems arise from many problems in machine learning ,such as generative modeling and adversarial learning. In general, finding the global Nash-equilibrium of a two-player zero-sum game is difficult when the objective function lacks convexity and concavity assumptions. In this talk, I will introduce a mean-field setting of the game problem and discuss some global convergence results of GDA for finding mixed equilibria on the space of probability measures.

00193 (2/3) : 5C @E503 [Chair: Tim Roith]

## [00292] Gamma convergence of a nonlocal perimeter from adversarial machine learning

**Format :** Talk at Waseda University

**Author(s) :** Leon Bungert (University of Bonn)Kerrek Stinson (University of Bonn)

**Abstract :** Adversarial training is a robust machine learning method which seeks to compute a classifier which is stable with respect to adversarial attacks. Recent analysis has shown that adversarial training admits different reformulations, e.g., as distributionally robust optimization, multi-marginal optimal transport, or geometric regularization problem. In this last context, adversarial training is equivalent to regularized empirical risk minimization  $\min_{A \subset \mathbb{R}^d} \mathcal{R}_{\text{emp}}(A) + \varepsilon \text{Per}_\varepsilon(A)$  where a nonlocal perimeter  $\text{Per}_\varepsilon$  of the classifier is penalized. The nonlocality is parametrized with the so-called “adversarial budget”  $\varepsilon > 0$  which models the strength of the adversary. In this talk I will discuss local limits of this nonlocal perimeter as the adversarial budget goes to zero. Under generic conditions we prove Gamma convergence of  $\text{Per}_\varepsilon$  to a weighted local perimeter as  $\varepsilon \rightarrow 0$ . This is joint work with Kerrek Stinson from the University of Bonn.

## [00313] Provable Adversarial Robustness via Optimal Transport

**Format :** Talk at Waseda University

**Author(s) :** Muni Sreenivas Pydi (Université Paris Dauphine-PSL)

**Abstract :** In this talk, we explore the fundamental limits of adversarially robust classification using optimal transport. We give two characterizations of the best error: as an optimal transport cost between the true data distributions, and as the Bayes error of a minimax hypothesis test involving Wasserstein uncertainty sets. The first characterization leads to a recipe for finding the optimal classifier, and the second leads to the existence of a Nash equilibrium.

## [00277] Adversarial learning and the Wasserstein barycenter problem

**Format :** Talk at Waseda University

**Author(s) :** Matt Jacobs (Purdue University)

**Abstract :** In this talk, I will show that the adversarial training problem is equivalent to a generalized version of the Wasserstein barycenter problem. The connection between these problems allows us to completely characterize the optimal adversarial strategy and to bring in tools from optimal transport to analyze and compute optimal classifiers. We will then use these tools to better understand the regularizing effect of adversarial training.

## [00299] Optimal Adversarial Classification: geometry, regularity, and topology

**Format :** Talk at Waseda University

**Author(s) :** Ryan Murray (North Carolina State University)

**Abstract :** Classification is a fundamental task in data science and machine learning, and in the past ten years there have been significant improvements on classification tasks (e.g. via deep learning). However, recently there have been a number of works demonstrating that these improved algorithms can be "fooled" using specially constructed adversarial examples. In turn, there has been increased attention given to creating machine learning algorithms which are more robust against adversarial attacks.

In this talk I will discuss delicate mathematical and geometric information which can be inferred about optimal adversarial classifiers. In particular, I will describe types of available regularity theory, and draw connections with non-local isoperimetric problems which have been popular in the variational community. Time permitting, I will also discuss recent algorithmic advances which can detect and track topological changes induced by the presence of an adversary.

00193 (3/3) : 5D @E503 [Chair: Tim Roith]

## [00330] Adversarial flows

**Format :** Talk at Waseda University

**Author(s) :** Lukas Weigand (Friedrich-Alexander-Universität Erlangen-Nürnberg) Tim Roith (Friedrich-Alexander-Universität Erlangen-Nürnberg) Martin Burger (Friedrich-Alexander-Universität Erlangen-Nürnberg)

**Abstract :** The fast gradient method and the fast gradient sign method are two popular methods to generate adversaries of neural networks. Iterative applications of those methods yield differential equations, corresponding to  $p$ -curves of maximum slope in  $\mathbb{R}^d$  for the limit case  $p = \infty$ . We extend current analysis to this limit case, which allow us to generate distributional adversaries by corresponding  $\infty$ -curves of maximum slope in the  $\infty$ -Wasserstein space.

## [02000] Distributionally Robust Linear Predictors using the Max-Sliced Wasserstein Metric

**Format :** Talk at Waseda University

**Author(s) :** Cynthia Rush (Columbia University)

**Abstract :** We study the classical problem of predicting an outcome variable,  $Y$ , using a linear combination of a  $d$ -dimensional covariate vector,  $X$ . We provide conditions under which linear predictors that minimize the worst-case prediction error over a ball of distributions determined by a type of max-sliced Wasserstein metric are equivalent to linear predictors whose coefficients solve:  $\inf_{\beta} \beta \cdot (\mathbb{E}[Y - \langle \beta, X \rangle]^r)^{1/r} + \delta \|\beta\|$ , where  $r > 1$  and  $\delta > 0$  is a regularization parameter. A detailed analysis of the statistical properties of this metric yields a simple recommendation for the choice of regularization parameter. The suggested order of  $\delta$ , after a suitable normalization of the covariates, is typically  $d/n$ , up to logarithmic factors. Our recommendation is computationally straightforward to implement, pivotal, has provable out-of-sample performance guarantees, and does not rely on sparsity assumptions about the true data generating process.

This is joint work with Jose Montiel Olea, Amilcar Velez and Johannes Wiesel.

## [00352] Minimax results for Surrogate risks in Adversarial Learning

**Format :** Talk at Waseda University

**Author(s) :** Natalie Frank (NYU)

**Abstract :** Robustness to adversarial perturbations is of paramount concern in modern machine learning. One of the state-of-the-art methods for training robust classifiers is adversarial training, which involves minimizing a supremum-based surrogate risk. We prove a minimax theorem for this adversarial surrogate risk and discuss some of the algorithmic implications. Specifically, we use this minimax result to characterize the statistical consistency of surrogate risks in the adversarial setting.

## [00349] Robust second-order estimation algorithms

**Format :** Online Talk on Zoom

**Author(s) :** Po-Ling Loh (University of Cambridge)

**Abstract :** We provide a new computationally-efficient algorithm that finds estimators for the empirical risk minimization problem. We show that these estimators are robust for general statistical models. Our workhorse is a novel robust variant of Newton's method, and we provide conditions under which our version of Newton's method variant provides accurate estimators for general convex objectives.

# [00194] Recent Progress of Computational Electromagnetics

**Session Time & Room :** 1E (Aug.21, 17:40-19:20) @E705

**Type :** Proposal of Minisymposium

**Abstract :** This minisymposium will feature the recent advances and challenges in the field of computational electromagnetics. The topics covered in the minisymposium will include (but be not limited to) novel numerical methods and techniques for solving electromagnetic partial differential equations, e.g., use of the extended finite element methods in eddy-current problem, and balancing domain decomposition method for large-scale parallel computation for electromagnetic fields.

**Organizer(s) :** Takeshi Mifune, Tetsuji Matsuo, Takeshi Iwashita

**Classification :** 65Mxx, 65Fxx

**Minisymposium Program :**

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00194 (1/1) : 1E @E705 [Chair: Takeshi Mifune]

## [03979] Application of POD to solve non linear magnetoquasistatic FE problems

**Format :** Online Talk on Zoom

**Author(s) :** Stephane Clenet (AMValorArts et Métiers Science and Technology)Thomas Henneron (University of Lille)Theo Delagnes (EdF R&D)

**Abstract :** The Finite Element (FE) method is widely used to build accurate models of electrical devices but leads to the solution of large scale equation systems. To overcome this issue, model order reduction methods, like Proper Orthogonal Decomposition (POD), can significantly reduce the size of the equation system. In the presentation, the principles of POD method will be presented and how it can be applied to reduce FE model of non linear magnetoquasistatics problems. Application examples (transformers, electrical machines....) are given to illustrate the effectiveness of the POD method and also its limitations.

## [04030] BDD-DIAG Preconditioner of the Interface Problem for Magnetostatic Domain Decomposition Analysis

**Format :** Online Talk on Zoom

**Author(s) :** Hiroshi Kanayama (Japan Women's University)Masao Ogino (Daido University)Shin-ichiro Sugimoto (Hachinohe Institute of Technology)Kaworu Yodo (Insight Inc.)

**Abstract :** An iterative domain decomposition method is proposed for numerical analysis of 3-Dimensional linear magnetostatic problems taking the magnetic vector potential as an unknown function. The iterative domain decomposition method is combined with the Preconditioned Conjugate Gradient procedure and the Hierarchical Domain Decomposition Method which is adopted in parallel computing. Our previously employed preconditioner was the Neumann-Neumann preconditioner. Numerical results showed that the method was only effective for smaller problems. In this paper, we consider its improvement with the Balancing Domain Decomposition DIAGONal scaling (BDD-DIAG) preconditioner.

## [04666] Reduced Order Modeling of a Cage Induction Motor with Skewed Rotor Slots

**Format :** Online Talk on Zoom

**Author(s) :** Yasuhito Takahashi (Doshisha University)Koji Fujiwara (Doshisha University)Kengo Sugahara (Kindai University)Tetsuji Matsuo (Kyoto University)

**Abstract :** A method for deriving a reduced-order model of cage induction motors with skewed rotor slots is investigated based on the multiport Cauer ladder network method. The features of the several formulations for the skewed rotor are discussed, in which the continuity of the bar currents and the space harmonics included in the air-gap flux density waveform are treated differently. The effectiveness of the developed methods is verified from the viewpoints of computational accuracy and cost.

## [05040] Introducing extended finite element approaches in eddy currents analysis

**Format :** Talk at Waseda University

**Author(s) :** Shingo Hiruma (Kyoto University)

**Abstract :** In recent years, the evaluation of eddy current losses caused by harmonic components in power supplies has become increasingly important. However, the conventional finite element method requires the conductor region to be divided into fine elements, which results in high computational cost. In this study, we apply the extended finite element approach to high-frequency eddy current analysis and show that accurate analysis can be performed with low computational cost.

## [00196] Recent development of mathematical geophysics

**Session Time & Room :** 3D (Aug.23, 15:30-17:10) @G710

**Type :** Proposal of Minisymposium

**Abstract :** The purpose of this minisymposium is to interact with mathematicians working on geophysics with various recent topics: large time behavior of solutions, machine learning approach, flow behavior on manifolds and meteorological analysis. These each topics have long research history. However, the tendency of the recent studies seems to be a broader point of view, not only from each own research field but also from an interdisciplinary perspective.

**Organizer(s) :** Tsuyoshi Yoneda

**Classification :** 35Q86, 76U05, 35Q30, 37N10, 76D03

**Minisymposium Program :**

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00196 (1/1) : 3D @G710 [Chair: Tsuyoshi Yoneda]

## [01262] Global solutions for rotating MHD equations in the critical space

**Format :** Talk at Waseda University

**Author(s) :** Ryo Takada (The University of Tokyo)Keiji Yoneda (Kyushu University)

**Abstract :** We consider the initial value problem for the incompressible rotating magnetohydrodynamics equations in  $\mathbb{R}^3$ . We prove the unique existence of global solutions for large initial data in the scaling critical space  $\dot{H}^{\frac{1}{2}}(\mathbb{R}^3)$  when the rotation speed is sufficiently high. In order to control large magnetic fields, we introduce a modified linear solution for the velocity, and show its smallness in a suitable space-time norm by means of the dispersive effect of the Coriolis force.

## [02684] Multi-scale interaction of tropical weather in a simplified three-dimensional model

**Format :** Talk at Waseda University

**Author(s) :** Daisuke Takasuka (University of Tokyo)

**Abstract :** In the tropics, various kinds of weather systems are spontaneously realized, as represented by mesoscale convective systems, equatorial waves, the Madden-Julian oscillation ( $\text{MJO}$ ). They interact with each other through moist processes, wave-mean-flow interaction, and so on. As an example of this, we will present a non-linear multi-scale process in the MJO initiation, which involves the mean tropical circulations and equatorial waves, using a simplified three-dimensional fluid dynamical model.

## [00606] Eigenvalue Problem for Perturbation Operator of Two-jet Kolmogorov Type Flow

**Format :** Talk at Waseda University

**Author(s) :** Tatsu-Hiko Miura (Hirosaki University)

**Abstract :** We consider the linear stability of the two-jet Kolmogorov type flow which is a stationary solution to the vorticity equation on the unit sphere given by the zonal spherical harmonic function of degree two. Using the mixing structure of the two-jet Kolmogorov type flow, we show that the perturbation operator does not have eigenvalues except for zero. As an application, we also prove the occurrence of the enhanced dissipation in the linearized setting.

## [00377] On the physics-informed neural networks approximating the primitive equations

**Format :** Online Talk on Zoom

**Author(s) :** Quyuan Lin (University of California, Santa Barbara)Ruimeng Hu (University of California, Santa Barbara)Alan Raydan (University of California, Santa Barbara)Sui Tang (University of California, Santa Barbara)

**Abstract :** Large scale dynamics of the oceans and the atmosphere are governed by the primitive equations (PEs). Due to the nonlinearity and nonlocality, the numerical study of the PEs is in general a hard task. In this talk, I will introduce physics-informed neural networks (PINNs) to tackle this challenge, and show the theoretical error estimates and the results from numerical experiments that confirm the reliability of PINNs.

## [00201] Data-Driven Methods for Rough PDEs

**Session Time & Room :**

00201 (1/3) : 2C (Aug.22, 13:20-15:00) @E705

00201 (2/3) : 2D (Aug.22, 15:30-17:10) @E705

00201 (3/3) : 2E (Aug.22, 17:40-19:20) @E705

**Type :** Proposal of Minisymposium

**Abstract :** Recently there has been an increased interest in applying data driven methods to learn partial differential equations (PDEs). For example, operator learning has been developed to learn maps between infinite-dimensional function spaces and has shown success in the context of smooth PDEs. However, these methods perform poorly in areas where PDEs are less well-behaved; for instance, when equations are parameterized by non-smooth functions or when the PDE involves stochasticity. This mini-symposium invites experts on novel methods for learning stochastic and ill-conditioned multiscale PDEs. Topics will include numerical methods for SPDEs, learning in multiscale settings, and advances in operator learning.

**Organizer(s) :** Matthieu Darcy, Edoardo Calvello

**Classification :** 65Mxx, 60Gxx, 35Rxx, 37Hxx

**Minisymposium Program :**

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00201 (1/3) : 2C @E705 [Chair: Margaret Trautner]

## [04969] Operator Learning by Regressing PDEs

**Format :** Talk at Waseda University

**Author(s) :** Bamdad Hosseini (University of Washington)

**Abstract :** In this talk we will discuss a new approach towards operator learning by regression or discovery of the functional form the PDE. A simple, three step approach will be discussed that can be implemented using convenient, off-the-shelf kernel regression tools. Our approach naturally includes PDEs with unknown and variable coefficients and obtains competitive accuracy when training data is very scarce.

## [05235] Neural Operator for Discovering Physical Equations

**Format :** Talk at Waseda University

**Author(s) :** Paul Bogdan (USC)Xiongye Xiao (USC)Gaurav Gupta (USC)Radu Victor Balan (UMD)

**Abstract :** We develop a multiwavelet-based neural operator learning architecture that compresses the associated operator's kernel using fine-grained multiwavelets. For the initial value problems, we propose an exponential neural operator scheme for efficiently learning the map between the initial condition and the activities at later times. To solve coupled partial differential equations, we propose the coupled multiwavelets operator learning scheme by decoupling the coupled integral kernels during the decomposition and reconstruction procedures in the Wavelet space.

## [05013] Neural Option Pricing for Rough Bergomi Model

**Format :** Talk at Waseda University

**Author(s) :** Guanglian Li (HKU )

**Abstract :** This research investigates pricing financial options based on the rough Bergomi model by neural SDEs. We propose an efficient approximation of sample paths using the sum of exponentials and implement the Wasserstein distance as a loss function for network training. The option pricing is entirely based on the traditional martingale theory.

Our experimental results indicate that the error of the option price can be bounded by the very Wasserstein distance attained during training.

## [05221] One shot learning of stochastic differential equations with kernel methods

**Format :** Talk at Waseda University

**Author(s) :** Matthieu Darcy (California Institute of Technology )Boumediene Hamzi (Johns Hopkins University)Giulia Livieri (Scuola Normale Superiore)Houman Owhadi (California Institute of Technology)Peyman Tavallali (Jet Propulsion Lab, NASA)

**Abstract :** We consider the problem of learning a Stochastic Differential Equations from one sample trajectory, a challenging problem as a single trajectory only provides indirect information on the unknown functions. We propose a kernel-based method that recovers the drift function  $f$  and the diffusion function  $\sigma$  via Maximum a Posteriori Estimation given the data. Additionally, we learn the kernels from data with randomized cross-validation. Numerical examples illustrate the efficacy and robustness of our method.

00201 (2/3) : 2D @E705 [Chair: Matthieu Darcy]

## [03744] GMsFEM based multiscale model learning

**Format :** Talk at Waseda University

**Author(s) :** Eric Chung (The Chinese University of Hong Kong)Yiran Wang (Purdue University)Shubin Fu (Eastern Institute for Advanced Study)

**Abstract :** In this talk, we present a deep learning based reduced order modeling method for stochastic flow problems in highly heterogeneous media. We aim to utilize supervised learning to build a reduced surrogate mapping from the stochastic parameter space that characterizes the possible highly heterogeneous media to the solution space of a stochastic flow problem. The research of Eric Chung is partially supported by the Hong Kong RGC General Research Fund (Projects: 14305222 and 14304021).

## [03131] Multilevel Picard Approximation Algorithm for Semi-linear Integro-differential Equations

**Format :** Talk at Waseda University

**Author(s) :** Ariel Neufeld (Nanyang Technological University)Sizhou Wu (Nanyang Technological University)

**Abstract :** We introduce a multilevel Picard approximation algorithm for semi-linear parabolic partial integro-differential equations (PIDEs). We prove that the numerical approximation scheme converges to the unique viscosity solution of the PIDE under consideration. To that end, we derive a nonlinear Feynman-Kac formula. Furthermore, we show that the algorithm does not suffer from the curse of dimensionality, i.e., the computational complexity of the algorithm is bounded polynomially in the dimension and the reciprocal of the prescribed accuracy.

## [03090] Exponentially Convergent Multiscale Finite Element Method

**Format :** Talk at Waseda University

**Author(s) :** Yixuan Wang (California Institute of Technology)

**Abstract :** Exponentially convergent multiscale finite element method (ExpMsFEM) for efficient model reduction of PDEs in heterogeneous media without scale separation and in high-frequency wave propagation is proposed. ExpMsFEM is built on the non-overlapped domain decomposition in the classical MsFEM while enriching the approximation space systematically to achieve a nearly exponential convergence rate regarding the number of basis functions.

## [05179] Learning Solutions to Elliptic PDEs with Discontinuous Multiscale Parameters

**Format :** Talk at Waseda University

**Author(s) :** Margaret Katherine Trautner (California Institute of Technology)

**Abstract :** Elliptic partial differential equations with discontinuous coefficients arise in modeling dynamics of solid materials. When these coefficients are also multiscale, homogenization theory eliminates the rapidly-varying stiff variable. The bottleneck of this approach is solving an associated cell problem whose discontinuous parameters make solving computationally expensive. Thus, we aim to learn the cell problem solution via data-driven means. In this talk, we describe rigorous theory underpinning these learning methods and numerical experiments that validate the theory.

00201 (3/3) : 2E @E705 [Chair: Edoardo Calvello]

## [04555] Recent Advances in Rigorous Koopmanism

**Format :** Talk at Waseda University

**Author(s) :** Matthew Colbrook (University of Cambridge)Qin Li (UW-Madison)Ryan Raut (University of Washington)Alex Townsend (Cornell University)

**Abstract :** Koopman operators are infinite-dimensional operators that globally linearize nonlinear dynamical systems, making their spectral information valuable for understanding dynamics. They have received considerable attention over the last decade, yet computing their spectral properties is a major challenge. I will present some recent advances in data-driven computation of Koopman spectral properties, including ResDMD and its analogue for stochastic dynamical systems. These new algorithms verifiably converge to the correct spectral properties (avoiding issues such as spectral pollution).

## [05147] Solving path-dependent PDEs with signature kernels

**Format :** Talk at Waseda University

**Author(s) :** Cristopher Salvi (Imperial College London)

**Abstract :** In talk I will introduce a kernel framework for solving path-dependent PDEs (PPDEs) leveraging signature kernels, a recently introduced class of kernels indexed on path space. The proposed method recast the original infinite dimensional optimisation problem to an optimal recovery problem that approximates the solution of a PPDE with an element of minimal norm in the (signature) reproducing kernel Hilbert space constrained to satisfy the PPDE at a finite collection of collocation paths. By the representer theorem, the optimisation has a unique, analytic solution expressed entirely in terms of simple linear algebra operations. I will discuss some motivating examples from rough volatility and present numerical results on option pricing under a rough Bergomi model.

## [05248] Kernel Methods for Rough PDEs

**Format :** Talk at Waseda University

**Author(s) :** Edoardo Calvello (California Institute of Technology )Ricardo Baptista (California Institute of Technology)Matthieu Darcy (California Institute of Technology )Houman Owhadi (California Institute of Technology)Andrew Stuart (California Institute of Technology)Xianjin Yang (California Institute of Technology)

**Abstract :** Following the promising success of kernel methods in solving non-linear partial differential equations (PDEs), we investigate the application of Gaussian process methods to solve PDEs with rough right-hand side. We introduce an optimal recovery scheme defined by a Reproducing Kernel Hilbert Space (RKHS) of functions of greater regularity than that of the PDE's solution. We illustrate the resulting theoretical framework for the recovery of solutions to the PDE and related numerical experiments.

# [00211] Mathematics of Geometric Deep Learning

**Session Time & Room :**

00211 (1/4) : 1C (Aug.21, 13:20-15:00) @E812

00211 (2/4) : 1D (Aug.21, 15:30-17:10) @E812

00211 (3/4) : 1E (Aug.21, 17:40-19:20) @E812

00211 (4/4) : 2C (Aug.22, 13:20-15:00) @E812

**Type :** Proposal of Minisymposium

**Abstract :** Geometric deep learning has important applications in the fields of quantum computing, 3D perception, molecular designs, and the discovery of mathematical theorems. It takes account of properties such as invariance and equivariance. Many existing structure-aware deep networks lack rigorous theoretical foundations of desired properties in modeling, such as network stability, interpretability, and efficient computation. This workshop will gather researchers from mathematics and computer sciences to provide a forum to establish diverse mathematical theories for geometric deep learning, such as harmonic analysis, algebraic topology, algebraic geometry, combinatorics, differential geometry, differential equations, graph theory, approximation theory, statistics, and theoretical computer science.

**Organizer(s) :** Yuguang Wang, Bingxin Zhou, Yuelin Wang

**Classification :** 68T07, 65T60, 05E45, 53Z05, 70F40

**Minisymposium Program :**

## [01563] Negative sampling for graph neural networks based on determinantal point processes

**Author(s)** : Junyu Xuan (University of Technology Sydney)

**Abstract** : Graph neural networks (GNNs) have become the de facto standard of a variety of graph-based applications. Most GNNs are built on a message-passing mechanism and only aggregate information from the first-order neighbours (positive samples), which may lead to over-smoothing, limited expressive power and over-squashing. However, beyond these neighbouring nodes, graphs have a large, dark, all-but forgotten world in which we find the non-neighbouring nodes (negative samples) that are helpful for representation learning.

## [01565] Spherical Framelets with Directionality for Spherical Neural Networks

**Author(s)** : Jianfei Li (City University of Hong Kong)Han Feng (City University of Hong Kong)Xiaosheng Zhuang (City University of Hong Kong)

**Abstract** : In this talk, we shall focus on the constructions and applications of directional framelets beyond the Euclidean domain, i.e., on the 2-sphere. We shall discuss their characterizations in terms of the affine systems. Fast algorithmic framelet transforms associated with the underlying filter banks or multiscale structures will be investigated. Moreover, based on our spherical framelets with directionality, we shall consider the development of spherical convolutional neural network (SNN) model for deep learning tasks.

## [01568] Some Applications of Hyperplane Arrangements in Deep Learning

**Author(s)** : Huan Xiong (HIT and MBZUAI)

**Abstract** : In this talk, we build some connections between hyperplane arrangements and Piecewise Linear Convolutional Neural Networks (PLCNNs), and use them to derive maximal and average numbers of linear regions for one-layer PLCNNs. Furthermore, we obtain upper and lower bounds for the number of linear regions of multi-layer PLCNNs. Our results suggest that deeper ReLU CNNs have more powerful expressivity than their shallow counterparts, while ReLU CNNs have more expressivity than fully-connected ReLU NNs per parameter.

## [01769] Machine Learning in Banach Spaces: A Black-box or White-box Method?

**Author(s)** : Qi Ye (South China Normal University)

**Abstract** : In this talk, we study the whole theory of regularized learning for generalized data in Banach spaces including representer theorems, approximation theorems, and convergence theorems. Specially, we combine the data-driven and model-driven methods to study the new algorithms and theorems of the regularized learning. Usually the data-driven and model-driven methods are used to analyze the black-box and white-box models, respectively. With the same thought of the Tai Chi diagram, we use the discrete local information of the black-box and white-box models to construct the global approximate solutions by the regularized learning. Our original ideas are inspired by the eastern philosophy such as the golden mean. The work of the regularized learning for generalized data provides another road to study the algorithms of machine learning including: 1. the interpretability in approximation theory, 2. the nonconvexity and nonsmoothness in optimization theory, 3. the generalization and overfitting in regularization theory. Moreover, based on the theory of the regularized learning, we will construct the composite algorithms combining the model-driven and data-driven methods for our current research projects of the big data analytics in education and medicine.

## [01857] Stable Hyperbolic Neural Networks for Graph Generation and Classification

**Author(s)** : Eric Qu (Duke Kunshan University)Dongmian Zou (Duke Kunshan University)

**Abstract** : The past few years have witnessed successful development of hyperbolic neural networks. However, they are known to suffer from instability in training. In this talk, we present two recent works that build novel hyperbolic layers for generation and classification tasks on tree-like and hierarchical-structured data. The first defines a stable hybrid AE-GAN model; the second defines a hyperbolic convolutional layer built upon pre-defined kernel points. We illustrate their competitiveness by showing extensive numerical results.

## [02110] Spectral-Inspired Graph Neural Networks

**Author(s)** : Teresa Huang (Johns Hopkins University)

**Abstract** : Message Passing Neural Networks (MPNNs) can suffer from expressivity issues like over-smoothing and over-squashing. To mitigate such issues, we propose PowerEmbed -- a simple layer-wise normalization technique to boost MPNNs. We show PowerEmbed can provably express the top-k leading eigenvectors of the graph operator, which prevents over-smoothing and is agnostic to the graph topology; meanwhile, it produces a list of representations ranging from local features to global signals, which avoids over-squashing.

## [02341] Generalization Capabilities of Graph Neural Networks

**Author(s)** : Gitta Kutyniok (LMU Munich)Sohir Maskey (LMU Munich)Ron Levie (Technion)Yunseok Lee (LMU Munich)

**Abstract** : The tremendous importance of graph structured data due to recommender systems, social networks, or biological applications led to the introduction of graph neural networks. One key question in machine learning is the ability of a learnt model to generalize to unknown data sets. In this talk, we will present several results on the generalization capabilities of graph neural networks, focussing on both message passing and spectral graph neural networks.

## [03411] On the stability of spectral graph filters and beyond

**Author(s)** : Xiaowen Dong (University of Oxford)

**Abstract** : Data collected in network domains, hence supported by an (irregular) graph rather than a (regular) grid-like structure, are becoming pervasive. Typical examples include gene expression data associated with a protein-protein interaction graph, or behaviours of a group of individuals in a social network. Graph-based signal processing and machine learning are recent techniques that have been developed to handle such graph-structured data and have seen applications in such diverse fields as drug discovery, fake news detection, and traffic prediction. However, a theoretical understanding of the robustness of these models against perturbation to the input graph domain has been lacking. In this talk, I will present our results on the stability bounds of spectral graph filters as well as other recent work on the robustness of graph machine learning models, which together will contribute to the deployment of these models in real-world scenarios.

00211 (3/4) : 1E @E812

## [03588] Geometric Diffusion Generative model for protein sequence design

**Author(s)** : Kai Yi (UNSW)

**Abstract** : Propose a new approach to protein sequence design using a diffusion generative model in geometric. This approach has the potential to improve protein properties and has implications for biotechnology and medicine. The method outperforms state-of-the-art methods on benchmark datasets.

## [03727] FoSR: First-order spectral rewiring for addressing oversquashing in GNNs

**Author(s)** : Guido Montufar (UCLA and MPI MiS)

**Abstract** : Graph neural networks (GNNs) are able to leverage the structure of graph data by passing messages along the edges of the graph. While this allows GNNs to learn features depending on the graph structure, for certain graph topologies it leads to inefficient information propagation and a problem known as oversquashing. This has recently been linked with the curvature and spectral gap of the graph. On the other hand, adding edges to the message-passing graph can lead to increasingly similar node representations and a problem known as oversmoothing. We propose a computationally efficient algorithm that prevents oversquashing by systematically adding edges to the graph based on spectral expansion. We combine this with a relational architecture, which lets the GNN preserve the original graph structure and provably prevents oversmoothing. We find experimentally that our algorithm outperforms existing graph rewiring methods in several graph classification tasks. This is work with Kedar Karhadkar and Pradeep Kr. Banerjee.

## [04482] DynG2G: An Efficient Stochastic Graph Embedding Method for Temporal Graphs

**Author(s)** : Mengjia Xu (Brown University & MIT)Apoorva Vikram Singh (National Institute of Technology)George Em Karniadakis (Brown University)

**Abstract** : Dynamic graph embedding has gained great attention due to its capability of learning low-dimensional graph embeddings for complex temporal graphs with high accuracy. However, recent advances mostly focus on learning node embeddings as deterministic "vectors" for static graphs, hence disregarding the key graph temporal dynamics and the

evolving uncertainty associated with node embedding in the latent space. We propose an efficient stochastic dynamic graph embedding method (DynG2G) that applies an inductive feed-forward encoder trained with node triplet energy-based ranking loss. Every node per timestamp is encoded as a time-dependent probabilistic multivariate Gaussian distribution in the latent space. We adopted eight benchmarks of different sizes and evolving dynamics (from slowly changing dynamics to rapidly varying multi-rate dynamics). Our experiments indicate that DynG2G achieves new state-of-the-art performance in capturing the temporal node embeddings and simultaneously predicting the evolving node embedding uncertainty, which plays a crucial role in quantifying the intrinsic dimensionality of the dynamical system over time. We also obtain a “universal” relation of the optimal embedding dimension  $L$  versus the effective dimensionality of uncertainty ( $D$ ). The  $L - D$  correlation provides a clear path for selecting the optimum embedding size adaptively per timestamp by  $L \geq D$ .

### [04999] On oversquashing and expressivity: can GNNs mix variables?

**Author(s)** : Francesco Di Giovanni (University of Cambridge)

**Abstract** : I discuss how Message Passing Neural Networks (MPNNs) model mixing among features in a graph. As a consequence of this approach, I show that MPNNs may need as many layers as the (largest) commute time to model strong mixing of distant nodes in a graph. This allows to derive a measure for over-squashing and to clarify how the latter limits the expressivity of MPNNs to learn functions with long-range interactions.

00211 (4/4) : 2C @E812

### [05074] Applied harmonic analysis and particle dynamics for designing neural message passing on graphs

**Author(s)** : Yuguang Wang (Shanghai Jiao Tong University)

**Abstract** : Graph representation learning has broad applications from recommendation systems to drug and protein designs. In this talk, I will talk about using harmonic analysis and particle systems to design useful neural message passing with theoretically guaranteed separability and efficient computation. These message passings are proved to have strictly positive lower bounded Dirichlet energy and thus to circumvent the oversmoothing problem appearing in many spatial GNNs, when the node features are indistinguishable as the network deepens.

### [05109] Geometric Deep Learning from a Topological Viewpoint

**Author(s)** : Cristian Bodnar (Microsoft Research)

**Abstract** : The multitude of applications where data is attached to spaces with non-Euclidean structure has driven the rise of the field of Geometric Deep Learning (GDL). Nonetheless, from many points of view, geometry does not always provide the right level of abstraction to study all the spaces that commonly emerge in such settings. For instance, graphs, by far the most prevalent type of space in GDL, do not even have a geometrical structure in the strict sense. In this talk, I will explore how we can take a (more general) topological perspective of the field with a focus on understanding and developing Graph Neural Network models.

### [05231] Ridgelet Transforms of Neural Network on Manifolds and Hilbert Spaces

**Author(s)** : Sho Sonoda (RIKEN AIP)

**Abstract** : Ridgelet transform is a pseudo-inverse operator of neural networks. Namely, given a function  $f \in L^2(\mathbb{R}^m)$ , the ridgelet transform  $R[f]$  describes how the network parameters should be distributed for the network to represent  $f$ . In this talk, I will explain a systematic scheme to derive the ridgelet transform by turning the network into a Fourier expression. As applications, we extend the scheme to networks on manifolds  $G/K$  and Hilbert spaces  $H$ , and derive their associated ridgelet transforms.

### [05341] Scattering Message Passing

**Author(s)** : Yuanhong Jiang (Shanghai JiaoTong University)

**Abstract** : Graph neural network (GNN) with message Passing scheme provides an elegant way to process graph data. However, the stability, oversmoothing and oversquashing problems commonly exist in current GNN models. We propose the message passing scheme with scattering transform which is proved theoretically to solve the above problems. In the numerical experiments, the scattering message passing has been validated to be effective compared to SOTA GNN models.

# [00215] Mathematical Advances in the nonlinear PDEs from physics

## **Session Time & Room :**

00215 (1/3) : 4E (Aug.24, 17:40-19:20) @G702

00215 (2/3) : 5B (Aug.25, 10:40-12:20) @G702

00215 (3/3) : 5C (Aug.25, 13:20-15:00) @G702

## **Type :** Proposal of Minisymposium

**Abstract :** The aim of this mini-symposium is to bring together experts in the area of nonlinear PDEs from physics, such as Euler-type equations and Boltzmann equation, to present their recent research results in theoretical analysis and applications in physics. In this mini-symposium, people are expected to exchange new ideas, to discuss challenging issues, to explore new directions and topics, and to foster new collaborations and connections.

**Organizer(s) :** Renjun Duan, Xianpeng Hu, Tong Yang

**Classification :** 35Q20, 35Q35, 35M10

## **Minisymposium Program :**

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00215 (1/3) : 4E @G702 [Chair: Tong Yang]

## [04052] Wave propagation and stabilization in the Boussinesq–Burgers system

### **Format :** Talk at Waseda University

**Author(s) :** Zhi-An Wang (The Hong Kong Polytechnic University )

**Abstract :** This talk will discuss the existence and stability of traveling wave solutions of the Boussinesq–Burgers system describing the propagation of bores. Assuming the fluid is weakly dispersive, we establish the existence of three different wave profiles by the geometric singular perturbation theory alongside phase plane analysis. We further employ the method of weighted energy estimates to prove the nonlinear asymptotic stability of the traveling wave solutions against small perturbations. The technique of taking antiderivative is utilized to integrate perturbation functions because of the conservative structure of the Boussinesq–Burgers system. Using a change of variable to deal with the dispersion term, we perform numerical simulations for the Boussinesq–Burgers system to showcase the generation and propagation of various wave profiles in both weak and strong dispersions. The numerical simulations not only confirm our analytical results, but also illustrate that the Boussinesq–Burgers system can generate numerous propagating wave profiles depending on the profiles of initial data and the intensity of fluid dispersion, where in particular the propagation of bores can be generated from the system in the case of strong dispersion.

## [03930] Hypersonic similarity for steady potential flows over a two dimensional wedge

### **Format :** Talk at Waseda University

**Author(s) :** jie kuang (Academy of Mathematics and Systems Science)wei xiang (city university of hong kong)Yongqian Zhang (Fudan University)

**Abstract :** We will talk about our recent results on the hypersonic similarity for the potential flow over a two-dimensional wedge. The convergence is obtained in  $BV \cap L^1$  spaces. Progress on related problems will be presented too.

## [05017] Stability theory for the linear symmetric hyperbolic system with general relaxation

### **Format :** Talk at Waseda University

**Author(s) :** Yoshihiro Ueda (Kobe University)

**Abstract :** In this talk, we study the dissipative structure for the linear symmetric hyperbolic system with general relaxation. If the relaxation matrix of the system has symmetric properties, Shizuta and Kawashima(1985) introduced the suitable stability condition, and Umeda, Kawashima and Shizuta(1984) analyzed the dissipative structure. On the other hand, Ueda, Duan and Kawashima(2012,2018) focused on the system with non-symmetric relaxation and got partial results. Furthermore, they argued the new dissipative structure called the regularity-loss type. In this situation, this talk aims to extend the stability theory introduced by Shizuta and Kawashima(1985) and Umeda, Kawashima and

Shizuta(1984) to our general system. Furthermore, we will consider the optimality of the dissipative structure. If we have time, I would like to discuss some physical models for its application and new dissipative structures.

## [00454] Stability of Riemann shock wave via the method of a-contraction of shifts

**Format :** Talk at Waseda University

**Author(s) :** Moon-Jin Kang (KAIST)

**Abstract :** I will present the so-called "a-contraction with shifts" method.

This method is quite useful in studying the stability of Navier-Stokes and Euler flows perturbed from Riemann solution containing a shock wave.

First, this method is energy based, and so allows us to seamlessly handle the composite wave of a viscous shock and rarefaction for its long-time behavior.

On the other hand, since the method can handle large perturbations of a viscous shock, and so provides the uniform stability of the shock w.r.t. the strength of viscosity, we can prove that the Riemann solution composed of a shock is stable and unique in the class of inviscid limits of solutions to the associated Navier-Stokes system.

00215 (2/3) : 5B @G702 [Chair: Xianpeng Hu]

## [03959] Polynomial tail solutions for Boltzmann equation in the whole space

**Format :** Talk at Waseda University

**Author(s) :** Renjun Duan (The Chinese University of Hong Kong)

**Abstract :** We are concerned with the Cauchy problem on the Boltzmann equation in the whole space. The goal is to construct global-in-time bounded mild solutions near Maxwellians with the perturbation admitting a polynomial tail in large velocities. The main difficulty to be overcome in case of the whole space is the polynomial time decay of solutions which is much slower than the exponential rate in contrast with the torus case.

## [02793] Analytic regularization effect for the spatially inhomogeneous Boltzmann equation

**Format :** Talk at Waseda University

**Author(s) :** Wei-Xi LI (Wuhan University)

**Abstract :** We verify in this work the spatially inhomogeneous Boltzmann equation with strong angular singularity will admit the analytic smoothing effect, just like its diffusive models such as the Landau and Fokker-Planck equations. To overcome the degeneracy in the spatial variable, a family of well-chosen vector fields with time-dependent coefficients will play a crucial role in the proof

## [04010] Dispersive limit of kinetic models for collisional plasma

**Format :** Talk at Waseda University

**Author(s) :** Zhu Zhang (The Hong Kong Polytechnic University) Tong Yang (The Hong Kong Polytechnic University)

**Abstract :** The motion of charged particles can be described by the Vlasov-Poisson-Boltzmann (VPB) system. Compared to the classical Boltzmann equation for dilute gases, solutions to VPB are expected to have dispersive behavior because of the dispersion mechanism on the dynamics of plasma in different scales of physical interest. By a formal spectrum analysis, we can observe asymptotic relations between VPB and some limiting dispersive equations in a suitable regime. Then we justify that the propagation of non-linear ions-acoustic waves are governed by the KdV equation. This is a joint work with T. Yang.

## [04067] Wave propagation and stabilization in the Boussinesq-Burgers system

**Format :** Talk at Waseda University

**Author(s) :** Xianpeng Hu (City University of Hong Kong) Anita Yang (The Chinese University of Hong Kong)

**Abstract :** In this talk, we will present the existence and stability of traveling wave solutions of the Boussinesq-Burgers system describing the propagation of bores. Assuming the fluid is weakly dispersive, we establish the existence of three different wave profiles by the geometric singular perturbation theory alongside phase plane analysis. We further employ the method of weighted energy estimates to prove the nonlinear asymptotic stability of the traveling wave solutions against small perturbations. The technique of taking antiderivative is utilized to integrate perturbation functions because of the conservative structure of the Boussinesq-Burgers system. Using a change of variable to deal with the dispersion term, we perform numerical simulations for the Boussinesq-Burgers system to showcase the generation and propagation of various wave profiles in both weak and strong dispersions. The numerical simulations not only confirm our analytical results, but also illustrate that the Boussinesq-Burgers system can generate numerous propagating wave profiles depending on the profiles of initial data and the intensity of fluid dispersion, where in particular the propagation of bores

can be generated from the system in the case of strong dispersion. The talk is based on a recent joint work with Prof. Zhan Wang and Prof. Kun Zhao.

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00215 (3/3) : 5C @G702 [Chair: Renjun Duan]

### [04667] Vacuum free boundary problems in ideal compressible MHD

**Format :** Talk at Waseda University

**Author(s) :** Tao Wang (Wuhan University)

**Abstract :** We present the joint works with Professor Yuri Trakhinin on the local well-posedness of vacuum free boundary problems in ideal compressible magnetohydrodynamics (MHD) with or without surface tension.

### [01253] Well-posedness of some free boundary problems in compressible fluids

**Format :** Talk at Waseda University

**Author(s) :** Wenbin Zhao (Peking University)

**Abstract :** In this talk, we will discuss some free boundary problems in compressible fluids. We derive the evolution equation of the free surface and identify the stability condition of the problem. This method gives a unified approach to treat both incompressible and compressible fluids.

### [04043] Long time instability of compressible symmetric shear flows

**Format :** Talk at Waseda University

**Author(s) :** Xianpeng Hu (City University of Hong Kong) Andrew Yang (City University of Hong Kong)

**Abstract :** It is well-known that at high Reynolds numbers, the linearized Navier-Stokes equations around the inviscid stable shear profile admit growing mode solutions due to the destabilizing effect of small viscosities. This phenomenon, which is related to Tollmien-Schlichting instability, has been rigorously justified by Grenier-Guo-Nguyen [Adv. Math. 292 (2016); Duke J. Math. 165 (2016)] on incompressible Navier-Stokes equations. In this work, we aim to construct the Tollmien-Schlichting waves for the compressible Navier-Stokes equations over symmetric shear flows in a channel. We will also discuss the effect of temperature fields on the stability of these shear flows.

## [00216] Recent Advances on interfaces dynamics modeling and simulation

**Session Time & Room :**

00216 (1/3) : 5B (Aug.25, 10:40-12:20) @A601

00216 (2/3) : 5C (Aug.25, 13:20-15:00) @A601

00216 (3/3) : 5D (Aug.25, 15:30-17:10) @A601

**Type :** Proposal of Minisymposium

**Abstract :** Dynamics of the interface, like deformation and reaction, play an important role in biology like cell aggregation, and industry like water-proof material. Modeling and simulation of the dynamics of the interface are challenging since multiphase-flow and multiphysics fields are evolved. Recently, machine learning-based methods like Neural networks are introduced to solve the obtained nonlinear coupled system more efficiently. The purpose of this symposium is to bring together researchers working on modeling, theory, and numerics for interface problems, to share the latest advances in the field, and to provide a forum for joint collaborations.

**Organizer(s) :** Huaxiong Huang, Shixin Xu

**Classification :** 92B05, 76T06, 65M60, 35Q35, 35Q92

**Minisymposium Program :**

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00216 (1/3) : 5B @A601 [Chair: Ping Lin]

### [01225] Solving elliptic interface problems using neural networks

**Format :** Talk at Waseda University

**Author(s) :** Ming-Chih Lai (National Yang Ming Chiao Tung University)

**Abstract :** In this talk, we shall introduce a series of neural network methodology for solving elliptic interface problems that comprise of variable-coefficient Poisson equation and Stokes equations with interfaces. There are three novel features in the present network; namely, (i) jump discontinuities are accurately captured, (ii) it is completely

shallow, comprising only one hidden layer, (iii) it is completely mesh-free so the problems in irregular domains with irregular interfaces can be handled easily. Numerical results show better accuracy than the traditional finite difference method such as the immersed interface method.

## [01276] Role of Cohesive Fiber-Fiber Interactions in Fibrin Networks

**Format :** Online Talk on Zoom

**Author(s) :** Zhiliang Xu (University of Notre Dame)

**Abstract :** A novel structural mechanism of fibrin clots' mechanical response to external tensile loads is tested using newly developed three-dimensional computational model. This mechanism, underlying local strain-stiffening of individual fibers as well as global stiffening of the entire network, is based on previously neglected nascent cohesive pairwise interactions between individual fibers (crisscrossing) in fibrin networks formed under tensile load. The computational model enabled us to study structural details and quantify mechanical effects of the fiber-fiber cohesive crisscrossing during stretching of fibrin gels at various spatial scales. The results show that the nascent cohesive crisscrossing of fibers in stretched fibrin networks comprise an underappreciated important structural mechanism underlying the mechanical response of fibrin to (patho)physiological stresses that determine the course and outcomes of thrombotic and hemostatic disorders.

## [01217] Variational Lagrangian schemes for interface problems

**Format :** Online Talk on Zoom

**Author(s) :** Yiwei Wang (University of California, Riverside)Chun Liu (Illinois Institute of Technology)

**Abstract :** In this talk, we present a systematic framework for deriving variational numerical methods for generalized diffusions and gradient flows. The numerical framework is based on the energy-dissipation law, which describes all the physics and the assumptions in each system and can combine different types of spatial discretizations including Eulerian, Lagrangian, and particle-based approaches. The resulting semi-discrete equation inherits the variational structures from the continuous energy-dissipation law. We apply such an approach to construct variational Lagrangian schemes to several interface problems, including the Allen-Cahn type phase-field models and the porous medium equation. Numerical examples show the advantages of the variational Lagrangian schemes in capturing thin diffuse interfaces and free boundaries. This is joint work with Professor Chun Liu.

## [01256] Helical organization of DNA-like liquid crystal filaments in cylindrical viral capsids

**Format :** Online Talk on Zoom

**Author(s) :** Pei Liu (Florida Institute of Technology)

**Abstract :** We study equilibrium configurations of ds-DNA in a cylindrical viral capsid. The state of the encapsitated DNA consists of a disordered inner core enclosed by an ordered outer region, next to the capsid wall. The DNA configuration is described by a unit helical vector field, tangent to an associated center curve, passing through properly selected locations. We postulate an expression for the energy of the encapsulated DNA based on that of columnar chromonic liquid crystals. A thorough analysis of the Euler--Lagrange equations yields multiple solutions. We demonstrate that there is a trivial, non-helical solution, together with two solutions with nonzero helicity of opposite sign. Using bifurcation analysis, we derive the conditions for local stability and determine when the preferred coiling state is helical. The bifurcation parameters are the ratio of the twist versus the bend moduli of DNA and the ratio between the sizes of the ordered and the disordered regions.

00216 (2/3) : 5C @A601 [Chair: Ming-Chih Lai]

## [01231] A phase-field model and an energy-law preserving method for vesicles

**Format :** Talk at Waseda University

**Author(s) :** Ping Lin (University of Dundee)

**Abstract :** We will first show how to develop a thermodynamically consistent phase field model for the binary incompressible (quasi-incompressible) fluid. We then show how to apply the idea to model vesicle motions and deformations through a narrowed channel. We will also introduce a Lennard-Jones type of interaction potential for vesicle-vesicle and vesicle-channel wall interactions. An energy law preserving computational method is then developed for the model. A few computational examples including vesicle-wall and multi-vesicle interactions will be presented to demonstrate the model and the computational method.

**[01214] Free boundary problems in cardiovascular diseases****Format :** Talk at Waseda University**Author(s) :** Wenrui Hao (Penn State University)**Abstract :** I will present several free boundary problems based on the pathophysiology of cardiovascular disease. As an example, a mathematical model of atherosclerosis, based on this modeling approach, provides a personalized cardiovascular risk by solving a free boundary problem. Some interesting mathematical problems are also introduced by this new model to help us understand cardiovascular risk.**[05636] Buckling on Erythrocyte Membranes in Narrow Capillary Flows****Author(s) :** Deyun Liu (Shanghai Jiao Tong University)Kazuyasu Sugiyama (Osaka University)Xiaobo Gong (Shanghai Jiao Tong University)**Abstract :** Experiments and numerical simulations are conducted to understand the non-axisymmetric deformation of a single RBC in narrow tubes and the hydrodynamics associated. With decreasing capillary numbers, the stable deformation shapes of RBCs change from axisymmetric bullet shape to asymmetric deformation with buckling under the major effect of the negative pressure difference across cell membrane at the rear part of the deformed RBCs.**[01394] Machine Learning of Self Organization from Observation****Format :** Online Talk on Zoom**Author(s) :** Ming Zhong (Illinois Institute of Technology)**Abstract :** Self organization (also known as collective behaviors) can be found in studying crystal formation, aggregation of cells/animals, social behaviors of insects and humans, etc. It is a challenging task to understand such behaviors from the mathematical point of view. We offer a statistical/machine learning approach to understand these behaviors quantitatively from observation data; moreover, our learning approach can aid in validating and improving the modeling of collective behaviors.

We develop a learning framework to derive physically meaningful models to explain self organization from observation. We also investigate the steady state properties of our learned models, and extend the learning framework to include more complicated structures. We extend the learning approach to infer dynamical models for agents constrained on Riemannian manifolds. We further improve our learning capability to infer interaction feature variables as well as interaction kernels. We even study the effectiveness of our learning method on the NASA Jet Propulsion Laboratory's modern Ephemerides. Upon careful inspection of our model, we discover that it even captures portion of the general relativity effects. A complete learning theory on second-order systems is presented, as well as two new models on emergence of social hierarchy and combination of flocking and synchronization.

00216 (3/3) : 5D @A601 [Chair: Shixin Xu]

**[01249] A phase field model for droplets suspended in electrolyte solution****Format :** Talk at Waseda University**Author(s) :** Yuzhe Qin (Shanxi University)Huaxiong Huang (Beijing Normal University, Zhuhai)Shixin Xu (Duke Kunshan University)Zilong Song (Utah State University)**Abstract :** In this talk, we consider modeling the deformation of droplets suspended in electrolyte solution with the phase field method. Firstly, we derive the Poisson-Nernst-Planck-Navier-Stokes phase field model based on energy variational approach method. Secondly, we accomplish the asymptotic analysis for our model after nondimensionalizing the system and the sharp interface limits of our proposed model is consistent to the sharp interface model. We take a series of numerical experiments to validate the correctness and effectiveness about our model.**[01220] A deterministic particle simulation for micro-macro viscoelastic flows****Format :** Talk at Waseda University**Author(s) :** Xuelian Bao (Beijing Normal University)Chun Liu (Illinois Institute of Technology)Yiwei Wang (University of California, Riverside)**Abstract :** We propose a deterministic particle-FEM discretization to micro-macro models of dilute polymeric fluids, which combines a finite element discretization to the macroscopic fluid dynamic equation with a variational particle scheme to the microscopic Fokker-Planck equation. The discretization is constructed by a discrete energetic variational approach, and preserves the microscopic variational structure in the semi-discrete level. All numerical examples demonstrate the accuracy and robustness of the proposed deterministic particle-FEM approach.

## [01227] A Bubble Model for the Gating of Kv Channels

**Format :** Online Talk on Zoom

**Author(s) :** zilong song (Utah State University)ROBERT EISENBERG (Illinois Institute of Technology)Shixin Xu (Duke Kunshan University)Huaxiong Huang (York University)

**Abstract :** Voltage-gated Kv channels play fundamental roles in many biological processes. In this talk, we propose a bubble model coupled with a Poisson-Nernst-Planck (PNP) system to capture the key characteristics, particularly the delay in the opening of channels. The coupled PNP system is solved numerically by a finite-difference method and the solution is compared with an analytical approximation. The predicted ensemble average of the currents and the Cole-Moore delay is consistent with experimental observations.

## [00217] Integration of modeling and data analysis on molecular, cellular, and population dynamics in the life sciences

**Session Time & Room :**

00217 (1/3) : 2C (Aug.22, 13:20-15:00) @A511

00217 (2/3) : 2D (Aug.22, 15:30-17:10) @A511

00217 (3/3) : 2E (Aug.22, 17:40-19:20) @A511

**Type :** Proposal of Minisymposium

**Abstract :** Systems biology approaches that integrate heterogeneous biological data in quantitative mathematical models are expected to facilitate a comprehensive understanding of complex biological systems. This A3 (China-Japan-Korea) mini-symposium will bring together Asian mathematicians working in the field of mathematical modeling and data analysis to share their cutting-edge research results on dynamic phenomena at all levels from molecular and cellular to population.

**Organizer(s) :** Jae Kyoung Kim, Sungrim Seirin-Lee, Lei Zhang

**Classification :** 92-08, 92-10, 92B20

**Minisymposium Program :**

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00217 (1/3) : 2C @A511

## [01180] Mathematical Models of Plasmid Loss

**Author(s) :** Kresimir Josic (University of Houston)Jayson Cortez (University of Philippines at Los Banos)Amanda Alexander (University of Houston)Charilaos Giannitsis (Rice University)Oleg Igoshin (Rice University)

**Abstract :** Plasmids, extrachromosomal DNA elements, are found in most bacteria and confer benefits to their hosts. Most models suggest that plasmids are lost in barring strong selection. The ubiquity of plasmids thus presents a paradox. We developed a mathematical model of ColE1 plasmid copy number based on experimental findings. This allows us to relate the probability of plasmid loss to properties of the population and provide testable predictions about conditions under which plasmids are lost.

## [00813] Morphology of organoids using a multicellular phase-field model

**Author(s) :** Sakurako Tanida (The University of Tokyo)Kana Fuji (The University of Tokyo)Tetsuya Hiraiwa (The University of Tokyo, National University of Singapore)Makiko Nonomura (Nihon University)Masaki Sano (The University of Tokyo, Shanghai Jiaotong University)

**Abstract :** Organoids are self-organizing cells grown from stem cells in vitro. The organoid morphology is affected not only by genes but also by mechanical constraints due to the geometrical requirements to maintain the cell cluster. In this study, using a multicellular phase-field model, we examined the morphology when changing luminal fluid pressure and the minimum time of the cell cycle. Classifying the patterns by several indices, we discuss the mechanisms which generate the different patterns.

## [00720] Mind the gap:The extra-embryonic space is crucial geometric constraints regulating cell arrangement.

**Author(s)** : Sungrim Seirin-Lee (Kyoto University)Kazunori Yamamoto (Kanagawa Institute of Technology)Akatsuki Kimura (National Institute of Genetics)

**Abstract** : Imagine sitting at a meeting where the shape of the table and your place at it might impact how you get along with the other members. In multicellular systems, cells also communicate with adjacent cells to decide their positions and fates. Cellular arrangement in space is thus important for development. Orientation of cell division, cell-cell interaction, and geometric constraints are the three major factors that define cell arrangement. In particular, the details of geometric constraints are difficult to be revealed only in experiments and the contribution of local contour has been remained elusive. Here we developed a multicellular morphology model based on the phase-field method so that we can incorporate precise geometric constrains. We applied the model to examine cell arrangement in the 4-cell stage embryo of nematodes, and succeeded in reproducing cell arrangements observed in vivo, including an arrangement which has not been explained before. Our cell morphology model predicted that the amount of extra-embryonic space (ES), the empty space within the eggshell not occupied by embryonic cells, affects cell arrangement in a manner dependent on the local contour and the aspect ratio of the eggshell as well as the strength of cell adhesion. The prediction was validated experimentally as increasing the (ES) did change the cell arrangement in the *Cenorhabditis elegans* embryo. Overall, our analyses characterized the roles of new geometrical contributors, namely the amount of (ES) and the local contour, to cell arrangements. These factors should be considered in all multicellular systems, including human being.

### Reference

S. Seirin-Lee\*, K. Yamamoto, A. Kimura, The extra-embryonic space and the local contour are critical geometric constraints regulating cell arrangement (2022) Development. 149, dev200401.

## [03207] Test three different models for the Chlamydia developmental cycle with intrinsic noise

**Author(s)** : Jinsu Kim (POSTECH)

**Abstract** : Chlamydia is an intracellular bacterium that reproduces via an unusual developmental cycle such as late RB-EB conversion and heterogeneity of individual Chlamydia size. A key step is a conversion from a replicating form (RB) to an infectious form (EB), which occurs in a delayed and asynchronous manner. The regulatory mechanisms that control this developmental switch are unknown, but could potentially include extrinsic signals from the host cell or from other chlamydiae, or an intrinsic signal such as chlamydial cell size. In this presentation, we introduce three stochastic models, each based on a different regulatory mechanism. To test the models, we use the intrinsic noise of each model that can be estimated with statistical quantities measured experimentally. We found that all three models successfully reproduced the observed timing of RB-to-EB conversion and the growth curves of the developmental forms within an inclusion. However, only one model, based on the regulation of RB-to-EB conversion by RB size, was able to produce the positive correlation between the number of RBs and EBs and the monotonic time evolution of the coefficient of variation in the RB population.

00217 (2/3) : 2D @A511

## [03206] Network design principle for biological dual functions

**Author(s)** : Lei Zhang (Peking University)

**Abstract** : Biological systems are capable of performing complex functions with a remarkable degree of accuracy, reliability, and robustness. We postulate that behind the celebrated diversity of the biological world lie “universal” principles that emerge at various levels of organization. For example, many signaling systems execute adaptation under noisy circumstances, and transcriptional regulatory networks can robustly achieve accurate oscillation in the presence of biological noise. In this talk, we will explore two dual functions: one is adaptation and noise attenuation, and the other one is oscillation and noise attenuation. By analyzing and computing three-node or four-node networks, we reveal essential network design principles for biological dual functions, which can be utilized in synthetic biology.

## [03385] Density Physics-Informed Neural Network infers an arbitrary density distribution for non-Markovian system

**Author(s)** : Hyeontae Jo (Institute for Basic Science)Hyukpyo Hong (KAIST)Hyung Ju Hwang (Pohang University of Science and Technology)Won Chang (University of Cincinnati)Jae Kyung Kim (KAIST)

**Abstract** : In this talk, we developed Density-PINN (Physics-Informed Neural Networks), a method capable of estimating the probability density function embedded within a differential equation. While conventional PINNs have focused on determining the solutions or parameters of differential equations that can explain observed data, we introduce a specialized approach for estimating the probability density function contained within the equation. Specifically, when dealing with a limited number of stochastic time series as observed data, and where only the average of the data satisfies the solution of the differential equation, we have constructed a mean-generating model using

Variational Autoencoders. By applying our method to single-cell gene expression data from 16 promoters in response to antibiotic stress, we discovered that promoters with slower signaling initiation and transduction exhibit greater cell-to-cell heterogeneity in response intensity.

## [02263] Integrating different layers of biological data to enhance prediction

**Author(s)** : Suoqin Jin (Wuhan University)

**Abstract** : The rapid advances of single-cell technologies have been attracting more attention. Recently we made some efforts to enhance biological prediction and discovery from single-cell RNA sequencing. By integrating single-cell RNA-seq with single-cell epigenomic data, bulk data or prior knowledge, we were able to dissect cellular heterogeneity and communication more comprehensively, and prioritize clinically-relevant cell subsets and prognostic signatures, which cannot be fully explained by single-cell genomics only, and highlights the valuable role of data integration.

## [03677] Physics of Furrow Ingression in *C. elegans* Zygote

**Author(s)** : Masatoshi Nishikawa (Hosei University)

**Abstract** : Cleavage furrow ingression is asymmetric in the first cleavage of *Caenorhabditis elegans* zygote. The asymmetric ingression gives rise to the symmetry breaking in terms of dorsal-ventral axis establishment, but its underlying mechanisms are largely unexplored. We will demonstrate that the distribution of cortical tension generator in the contractile ring becomes asymmetric as the curvature change at the ingression site and cortical flow toward the ring, suggesting the feedback between cell shape, contractility and flow.

00217 (3/3) : 2E @A511

## [01465] Screening cell-cell communication in spatial transcriptomics via collective optimal transport

**Author(s)** : Yanxiang Zhao (George Washington University)

**Abstract** : Spatial transcriptomic technologies and spatially annotated single cell RNA-sequencing (scRNA-seq) datasets provide unprecedented opportunities to dissect cell-cell communication (CCC). How to incorporate the spatial constraints and other physical processes when inferring CCC computationally remains a major challenge. Here we present COMMOT to infer CCC in spatial transcriptomics accounting for the competition among different ligand and receptor species and cells or spots, and enforcing spatial constraints. A novel collective optimal transport method is developed to handle these complex interactions and constraints. Further downstream analysis tools on spatial signaling directions and signaling-regulated genes are then developed using machine learning models. We validate the method with simulation data and one spatially annotated scRNA-seq dataset. We show that COMMOT effectively infers spatial CCC using datasets by three popular spatial transcriptomic technologies. Finally, COMMOT reveals connections between CCC and skin development in a case study of human epidermal development. The method will have broad application in uncovering ligand-receptor mediated CCC using spatial genomics datasets.

## [04188] A Novel Tool for Enhanced Single-cell RNA Sequencing Data Preprocessing and Dimensionality Reduction

**Author(s)** : Hyun Kim (Institute for basic science)JaeKyoung Kim (Korea Advanced Institute of Science and Technology, Institute for basic science)Jong-Eun Park (Korea Advanced Institute of Science and Technology)Minseok Seo (Korea University)

**Abstract** : Single-cell RNA sequencing (scRNA-seq) has revolutionized various cellular research applications, including cellular phenotyping and gene regulatory network reconstruction. However, data analysis remains challenging due to sparsity, high dimensionality, bias, skewed data distribution, and technological noise. In addition, conventional preprocessing methods, such as log-normalization and user-driven dimensionality reduction techniques, often introduce subjectivity and signal distortion, leading to decreased data dimension accuracy. To address these limitations, we developed a novel tool that effectively filters out data noise and corrects signal distortion during preprocessing. This approach significantly improves the accuracy of dimensionality reduction and overcomes the drawbacks associated with current methodologies. Our solution was tested on 53 real and simulated datasets and demonstrated superior performance compared to ten widely-used tools, including Seurat, Scanpy, and Monocle3. The enhanced performance of our tool offers promise for advancing scRNA-seq data analysis and facilitating more accurate downstream analyses.

## [00602] Adaptive immune discrimination of antigen risks by predictive coding

**Author(s)** : Kana Yoshida (Graduate School of Biostudies, Kyoto University)Honda Naoki (Graduate School of Integrated Sciences for Life, Hiroshima University)

**Abstract** : Immune system induces appropriate responses depending on the risk of antigens: Strong responses to harmful antigens and weak or no responses to harmless antigens. To reveal the mechanism, we modeled T cell population dynamics with memory formation based on predictive coding. By the simulation, we found antigen

part\_1

concentration- and input rapidness- dependent discrimination between harmful and harmless antigens. Furthermore, we reproduced temporal change of discrimination as seen in the onset and therapy of allergy.

## [00220] Reaction-Diffusion Systems and Applications in life Sciences

### **Session Time & Room :**

00220 (1/3) : 5B (Aug.25, 10:40-12:20) @G601

00220 (2/3) : 5C (Aug.25, 13:20-15:00) @G601

00220 (3/3) : 5D (Aug.25, 15:30-17:10) @G601

**Type :** Proposal of Minisymposium

**Abstract :** In this minisymposium we will focus on recent progress about the theory and applications of reaction-diffusion systems. A special focus will be on the mathematical modelling and analysis for evolution systems with applications in biological, ecological, health and medical sciences such as modelling infectious diseases and tumor growth in life sciences. The minisymposium will invite experts in the field to report their recent results on these subjects.

**Organizer(s) :** Hong-Ming Yin, Takashi Suzuki, Yihong Du

**Classification :** 35K40, 35R30, 35R25

### **Minisymposium Program :**

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00220 (1/3) : 5B @G601 [Chair: Hong-Ming Yin]

## [01711] Propagation dynamics of the Fisher-KPP nonlocal diffusion equation with free boundary

**Format :** Talk at Waseda University

**Author(s) :** Yihong Du (University of New England)

**Abstract :** Propagation has been modelled by reaction-diffusion equations since the pioneering works of Fisher and Kolmogorov-Petrowski-Piskunov (KPP). Much new developments have been achieved in the past several decades on the modelling of propagation, with traveling wave and related solutions playing a central role. In this talk, I will report some recent results obtained with several collaborators on the Fisher-KPP equation with free boundary and "nonlocal diffusion", where the diffusion operator is given by a convolution integral instead of the traditional Laplacian operator. A key feature of this nonlocal equation is that the propagation may or may not be determined by traveling wave solutions. There is a threshold condition on the kernel function in the diffusion operator which determines whether the propagation rate is linear or superlinear in time, also known as accelerated spreading in the latter case, where the rate of spreading is not determined by traveling waves. For some typical kernel functions, sharp spreading rates will be presented.

## [03297] propagation phenomena of fractional diffusion equations

**Format :** Talk at Waseda University

**Author(s) :** Xing Liang (University of Science and Technology of China)

**Abstract :** In this talk, I will introduce our works on the propagation phenomena of fractional diffusion equations. The first part is about KPP-type equations in almost periodic media. We will show the existence of exponential speeds of propagation and a counterintuitive conclusion that faster diffusion yields slower propagation. The second part is about bistable and multi-stable equation in periodic media. We will show the existence of the traveling terrace and when the traveling terrace becomes a traveling wave.

## [02984] Sharp traveling waves for degenerate equations with time-delay: Fisher-KPP equations and Burgers equations

**Format :** Talk at Waseda University

**Author(s) :** Ming Mei (McGill University & Champlain College)

**Abstract :** In this talk, we are concerned with the degenerate diffusion equations with time-delay. The typical examples include Fisher-KPP equations and Burgers equations. The main issue is to investigate the structure of traveling waves, which are the sharp traveling waves with oscillations. The sharpness is caused by the degeneracy of diffusion, and oscillation is caused by the large time-delay.

**[03485] Accelerating propagation in a nonlocal model with periodic time delay****Format :** Talk at Waseda University**Author(s) :** Jian Fang (Harbin Institute of Technology)**Abstract :** In this talk, we investigate the accelerating propagation dynamics of a nonlocal population model with periodic time delay, which may arise from the study of stage-structured invasive species subject to seasonal successions. After establishing the fundamental solution of related linear equation, we obtain a sharp estimate for the solution level set.

00220 (2/3) : 5C @G601 [Chair: Yihong Du]

**[01484] Recent Progress on Reaction-Diffusion Systems and Applications in Life Sciences****Format :** Talk at Waseda University**Author(s) :** Hong-Ming Yin (Washington State University)**Abstract :** Reaction-diffusion equations and systems are the backbone of many mathematical models in biological, ecological, health and medical sciences. In this talk I will first give a short survey on some recent progress about the global solvability for general reaction-diffusion systems. Then I will focus on a class of nonlinear reaction-diffusion systems with balanced mass. Some new results will be reported in the talk. Finally, I will show how the general result is used to establish the global solvability for two models arising from life sciences.**[04053] Effect of density-dependent dispersal on the predator-prey system****Format :** Talk at Waseda University**Author(s) :** Zhi-An Wang (The Hong Kong Polytechnic University )**Abstract :** This talk is concerned with existence, non-existence and uniqueness of positive (coexistence) steady states to a predator-prey system with density-dependent dispersal. By our analysis results, we pinpoint the positive role of density-dependent dispersal on the predator-prey dynamics for the first time and show that the density-dependent dispersal is a beneficial strategy promoting the coexistence of species in the predator-prey system by increasing the chance of predator's survival.**[04100] Nonlinear Stefan problem with a certain class of multi-stable nonlinearity****Format :** Talk at Waseda University**Author(s) :** Hiroshi Matsuzawa (Kanagawa University)Yuki Kaneko (Kanto Gakuin University)Yoshio Yamada (Waseda University)**Abstract :** I will discuss the long-time dynamical behavior of solutions to a nonlinear Stefan problem for a reaction-diffusion equation with a positive bistable type nonlinearity. I will show that the asymptotic behavior of the solutions is classified into four cases: vanishing, small spreading, big spreading, and transition. In particular, I will show that for transition occurs, the solution converges to an equilibrium solution that is radially symmetric, radially decreasing, and centered at some point as  $t \rightarrow \infty$ .**[01531] Some results on a haptotaxis model of cancer invasion****Format :** Online Talk on Zoom**Author(s) :** Feng Dai ( Huazhong University of Science and Technology)**Abstract :** In this talk, we will report some results on a haptotaxis model of cancer invasion. Under appropriate regularity assumptions on initial data, the global solvability of the corresponding homogeneous Neumann initial-boundary value problem is established. In addition, an optimal control problem for this cancer invasion model with chemotherapy is investigated to balance the therapeutic benefits with its side effects.

00220 (3/3) : 5D @G601 [Chair: Zhi-an Wang]

**[05208] Basic Propagation Number****Format :** Talk at Waseda University**Author(s) :** Juan B Gutierrez (University of Texas at San Antonio)**Abstract :** In this talk, I present a framework that describes the necessary and sufficient conditions for propagation of one or more undesirable species, named here the nonconformist species, in a given environment when there is an intervention trying to counter their propagation. We assume that the dispersal of the nonconformist could be characterized by a reaction-diffusion process, whereas there is no spatial dependence for the action of the

countermeasures. I present a generalized method that can analyze an arbitrary number of nonconformist species and countermeasures.

## [00221] Analysis of Fluid Dynamics and Free Boundary Problems

### **Session Time & Room :**

00221 (1/3) : 1C (Aug.21, 13:20-15:00) @D404

00221 (2/3) : 1D (Aug.21, 15:30-17:10) @D404

00221 (3/3) : 1E (Aug.21, 17:40-19:20) @D404

### **Type :** Proposal of Minisymposium

**Abstract :** This mini-symposium will focus on the analysis of fluid dynamics and free boundary problems including the geometric evolution equations. We will put particular emphasis on the study of existence, uniqueness, regularity, global existence and stability, singularity formation of the modeling equations and the motion of free interfaces in Euclidean spaces or on manifolds. The study of fluid dynamics and free boundary problems have profoundly impacted many applied fields such as physics, biology and material sciences. Thus the analysis of these problems provides a critical and rigorous mathematical descriptions of the corresponding physical phenomena.

**Organizer(s) :** Changyou Wang, Yuanzhen Shao

**Classification :** 76N10, 35R35

### **Minisymposium Program :**

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00221 (1/3) : 1C @D404 [Chair: Yuanzhen Shao]

## [03643] Transonic flows and free boundary problems in gas dynamics

### **Format :** Talk at Waseda University

**Author(s) :** Dehua Wang (University of Pittsburgh)University of Pittsburgh)

**Abstract :** In this talk, the transonic flows and free boundary problems in gas dynamics will be considered. The existence and stability of solutions will be presented for transonic flows past an obstacle and in a nozzle.

## [03380] Regularity and asymptotics for porous medium equations in bounded domains

### **Format :** Talk at Waseda University

**Author(s) :** Tianling Jin (The Hong Kong University of Science and Technology)Xavier Ros-Oton (Universitat de Barcelona)Jingang Xiong (Beijing Normal University)

**Abstract :** We prove the optimal global regularity of nonnegative solutions to the porous medium equation in smooth bounded domains with the zero Dirichlet boundary condition after certain waiting time. This allows us to refine the asymptotics of solutions for large times. We establish faster rate of convergence and prove that the convergence holds in the regular topology.

## [03966] Energy concentration and weak stability in fluid dynamics

### **Format :** Talk at Waseda University

**Author(s) :** Xianpeng Hu (City University of Hong Kong)

**Abstract :** The weak stability is an important issue in fluid dynamics. We will discuss the mathematical understanding of concentration phenomena in the framework of weak solutions with either critical or subcritical energy. Two typical examples, including two dimensional incompressible Euler equations and compressible Navier-Stokes equations, will be discussed.

## [03949] On Ericksen-Leslie system with free boundary

### **Format :** Talk at Waseda University

**Author(s) :** Yong Yu (The Chinese University of Hong Kong)Chenyun Luo (The Chinese University of Hong Kong)Kaihui Luo (The Chinese University of Hong Kong)

**Abstract :** In this talk, we discuss a 3D simplified Ericksen-Leslie system subjected to the free boundary condition with surface tension. Dynamical stability of the classical planar wave solutions will also be addressed when the liquid crystal droplet is thin.

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00221 (2/3) : 1D @D404 [Chair: Changyou Wang]

## [00618] L1 maximal regularity and its application to the Navier-Stokes equations

**Format :** Talk at Waseda University

**Author(s) :** Yoshihiro Shibata (Department of Mathematics, Waseda University)

**Abstract :** I will talk about the L1 maximal regularity theorem to the Stokes equations and its application to free boundary problem for the Navier-Stokes equations.

## [03780] Fluid flow on surfaces

**Format :** Talk at Waseda University

**Author(s) :** Gieri Simonett (Vanderbilt University) Mathias Wilke (Martin-Luther-Universität Halle-Wittenberg)

**Abstract :** I will consider the motion of an incompressible viscous fluid on compact surfaces without boundary.

Local in time well-posedness is established in the framework of  $L_p L_q$  maximal regularity for initial values in critical spaces.

It will be shown that the set of equilibria consists exactly of the Killing vector fields. Each equilibrium is stable and any solution starting close to an equilibrium converges at an exponential rate to a (possibly different) equilibrium. In case the surface is two-dimensional, it will be shown that any solution with divergence free initial value in  $L_2$  exists globally and converges to an equilibrium.

## [04880] The Curve Shortening Flow for Immersed Curves

**Format :** Talk at Waseda University

**Author(s) :** Patrick Guidotti (UC Irvine)

**Abstract :** We will revisit and study the curve shortening flow for immersed curves and its numerical computation.

## [03690] On a thermodynamically consistent model for magnetoviscoelastic fluids in 3D

**Format :** Talk at Waseda University

**Author(s) :** Hengrong Du (Vanderbilt University) Yuanzhen Shao (University of Alabama) Gieri Simonett (Vanderbilt University)

**Abstract :** In this talk, we consider a system of equations that model a non-isothermal magnetoviscoelastic fluid, which is thermodynamically consistent. The system is analyzed by means of the  $L^p$ -maximal regularity theory. First, we will discuss the local existence and uniqueness of a strong solution. Then it will be shown that a solution initially close to a constant equilibrium exists globally and converges to a (possibly different) constant equilibrium. Finally, we will show that every solution that is eventually bounded in the topology of the natural state space exists globally and converges to the set of equilibria.

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00221 (3/3) : 1E @D404 [Chair: Yuanzhen Shao]

## [04664] On some contact angle problems in fluid dynamics

**Format :** Online Talk on Zoom

**Author(s) :** Mathias Wilke (Martin-Luther-University Halle-Wittenberg)

**Abstract :** In this talk, we consider some contact angle problems for the dynamic of fluids and discuss several topics such as existence and uniqueness of solutions as well as their qualitative behaviour.

## [00258] The relativistic Euler equations with a physical vacuum boundary

**Format :** Talk at Waseda University

**Author(s) :** Marcelo Mendes Disconzi (Vanderbilt University)

**Abstract :**

We consider the relativistic Euler equations with a physical vacuum boundary and an equation of state  $p(\varrho) = \varrho^\gamma$ ,  $\gamma > 1$ . We establish the following results. i. local well-posedness in the Hadamard sense, i.e., local existence, uniqueness, and continuous dependence on the data; ii. low regularity solutions: our uniqueness result holds at the level of Lipschitz velocity and density, while our rough solutions, obtained as unique limits of smooth solutions, have regularity only a half derivative above scaling; iii. stability: our uniqueness in fact follows from a more general result, namely, we show that a certain nonlinear functional that tracks the distance between two solutions, in part by measuring the distance between their respective boundaries, is propagated by the flow; iv. we establish sharp, essentially scale invariant energy estimates for solutions; v. we establish a sharp continuation criterion, at the level of scaling, showing that solutions can be

part\_1

continued as long as the velocity is in  $L_t^1 Lip_x$  and a suitable weighted version of the density is at the same regularity level. This is joint work with Mihaela Ifrim and Daniel Tataru.

## [00223] Stochastic optimization and stochastic variational inequalities

**Session Time & Room :** 3D (Aug.23, 15:30-17:10) @A201

**Type :** Proposal of Minisymposium

**Abstract :** Stochastic optimization and stochastic variational inequalities are important mathematical tools for decision-making problems and equilibrium problems under uncertainty. This mini-symposium brings several researchers in stochastic optimization and stochastic variational inequalities together and offers an opportunity to discuss the latest developments.

**Organizer(s) :** Hailin Sun, Chao Zhang

**Classification :** 90C15, 90C33

**Minisymposium Program :**

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00223 (1/1) : 3D @A201 [Chair: Chao Zhang]

### [02880] Dynamic Stochastic Projection Method for Multistage Stochastic Variational Inequalities

**Format :** Talk at Waseda University

**Author(s) :** Hailin Sun (Nanjing Normal University)Bin Zhou (Nanjing Normal University)Jie Jiang (Chongqing University)

**Abstract :** Stochastic approximation (SA) type methods have been well studied for solving single-stage stochastic variational inequalities (SVIs). This paper proposes a dynamic stochastic projection method (DSPM) for solving multistage SVIs. In particular, we investigate an inexact single-stage SVI and present an inexact stochastic projection method (ISPM) for solving it. Then we give the DSPM to a three-stage SVI by applying the ISPM to each stage. We show that the DSPM can achieve an  $\mathcal{O}(\frac{1}{\epsilon^2})$  convergence rate regarding the total number of required scenarios for the three-stage SVI. We also extend the DSPM to the multistage SVI when the number of stages is larger than three. The numerical experiments illustrate the effectiveness and efficiency of the DSPM.

### [02891] A two-stage stochastic variational inequality model

**Format :** Talk at Waseda University

**Author(s) :** Min Li (Beijing Jiaotong University)Chao Zhang (Beijing Jiaotong University)Mingxv Ding (Beijing Jiaotong University)Ruipu Lv (Beijing Jiaotong University)

**Abstract :** This paper first proposes a new nonsmooth two-stage stochastic equilibrium model of medical supplies in epidemic management. The first stage addresses the storage in the pre-disaster phase, and the second stage focuses on the dynamic distribution in the post-disaster phase. The uncertainties are the numbers of infected people treated in multiple hospitals. The model is further approximated and transformed to a monotone two-stage stochastic variational inequality (SVI) model that is computationally tractable.

### [02899] Discrete approximation for two-stage stochastic variational inequalities

**Format :** Talk at Waseda University

**Author(s) :** Jie Jiang (Chongqing University)Hailin Sun (Nanjing Normal University)

**Abstract :** In this paper, the discrete approximation of two-stage stochastic variational inequalities has been investigated when the second stage problem has multiple solutions. First, a discrete approximation scheme is given by a series of models with the aid of merit functions. After that, the convergence relationships between these models are analysed, which therefore yields the convergence guarantee of the proposed discrete approximation scheme. Finally, we use the well-known progressive hedging algorithm to report some numerical results and to validate the effectiveness of the discrete approximation approach.

## [05136] Iteratively sampling scheme for stochastic optimization with variable number sample path

**Format :** Online Talk on Zoom

**Author(s) :** Dali ZHANG (Shanghai Jiao Tong University) Shuang HAO (Shanghai Jiao Tong University) Ming Dong (Shanghai Jiao Tong University)

**Abstract :** Optimal search methods are proposed for solving optimization problems with analytically unobtainable objectives. This paper proposes a method by incorporating sampling schemes into the directional direct search with variable number sample path and investigates its effectiveness in solving stochastic optimization problems. We also explore the conditions on sample sizes at each iteration under which the convergence in probability can be guaranteed. Finally, a set of benchmark problems are numerically tested to show the effectiveness in different sampling schemes.

## [00232] Theoretical foundations and algorithmic innovation in operator learning

**Session Time & Room :**

00232 (1/3) : 2C (Aug.22, 13:20-15:00) @E704

00232 (2/3) : 2D (Aug.22, 15:30-17:10) @E704

00232 (3/3) : 2E (Aug.22, 17:40-19:20) @E704

**Type :** Proposal of Minisymposium

**Abstract :** Many interesting phenomena in science and engineering involve operators mapping functions to functions. The application of data-driven tools from machine learning to scientific computing has thus given rise to the rapidly emerging field of operator learning. Despite encouraging practical successes, our understanding of these methods is still in its infancy, leaving important open questions to be addressed, including approximation guarantees, learning in data-scarce regimes, and understanding the limitations of current approaches and overcoming them. This minisymposium brings together researchers at the intersection of machine learning, approximation theory and PDEs to discuss theoretical foundations and recent algorithmic developments in this field.

**Organizer(s) :** Samuel Lanthaler, Jakob Zech

**Classification :** 65M99, 65N99, Machine Learning

**Minisymposium Program :**

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00232 (1/3) : 2C @E704 [Chair: Jakob Zech]

## [03323] BelNet: basis enhanced learning, a mesh-free neural operator

**Format :** Online Talk on Zoom

**Author(s) :** zecheng zhang (Carnegie Mellon University) Wing Tat Leung (City University Hong Kong) Hayden Schaeffer (UCLA)

**Abstract :** Operator learning trains a neural network to map functions to functions. An ideal operator learning framework should be mesh-free in the sense that the training does not require a particular choice of discretization for the input functions, allows for the input and output functions to be on different domains, and is able to have different grids between samples. We propose a mesh-free neural operator for solving parametric partial differential equations. The basis enhanced learning network (BelNet) projects the input function into a latent space and reconstructs the output functions. In particular, we construct part of the network to learn the "basis" functions in the training process. This generalized the networks proposed in Chen and Chen's universal approximation theory for the nonlinear operators to account for differences in input and output meshes. Through several challenging high-contrast and multiscale problems, we show that our approach outperforms other operator learning methods for these tasks and allows for more freedom in the sampling and/or discretization process.

## [01354] The curse of dimensionality in operator learning

**Format :** Talk at Waseda University

**Author(s) :** Samuel Lanthaler (California Institute of Technology)

**Abstract :** Neural operator architectures employ neural networks to approximate operators between Banach spaces of functions. We show that for general classes of operators, which are characterized only by their Lipschitz- or  $C^r$ -regularity, operator learning with neural operators suffers from a curse of dimensionality related to the infinite-dimensional input and output function spaces. This curse, made rigorous in this work, is characterized by an exponential lower complexity bound: in order to achieve approximation accuracy  $\epsilon$ , the number of tunable parameters generally has

to scale exponentially in  $\epsilon^{-1}$ . This negative result is applicable to a wide variety of existing neural operators, including DeepONet, the Fourier neural operator and PCA-Net. It is then shown that the general curse of dimensionality can be overcome for operators possessing additional structure, going beyond regularity. This is illustrated for the solution operator of the Hamilton-Jacobi equation.

## [05247] Score-based Diffusion Models in Function Space

**Format :** Talk at Waseda University

**Author(s) :** Nikola Kovachki (NVIDIA)

**Abstract :** We present a generalization of score-based diffusion models to function space by perturbing functional data via a Gaussian process at multiple scales. We obtain an appropriate notion of score by defining densities with respect to Gaussian measures and generalize denoising score matching. We then define the generative process by integrating a function-valued Langevin dynamic. We show that the corresponding discretized algorithm generates accurate samples at a fixed cost that is independent of the data discretization.

## [04771] Deep Learning Theories for Problems with Low-Dimensional Structures

**Format :** Talk at Waseda University

**Author(s) :** Hao Liu (Hong Kong Baptist University)Minshuo Chen (Princeton University)Siawpeng Er (Georgia Institute of Technology)Haizhao Yang (University of Maryland College Park)Tong Zhang (he Hong Kong University of Science and Technology)Tuo Zhao (Georgia Institute of Technology)Wenjing Liao (Georgia Institute of Technology)

**Abstract :** Deep neural networks have demonstrated a great success on many applications, especially on problems with high-dimensional data sets. However, most existing theories are cursed by data dimension. To mitigate the curse of dimensionality, we exploit the low-dimensional structures of data set and establish theoretical guarantees with a fast rate that is only cursed by the intrinsic dimension of the data set. This presentation addresses our recent work on function approximation and operator learning.

00232 (2/3) : 2D @E704 [Chair: Samuel Lanthaler]

## [04076] Local approximation of operators

**Format :** Talk at Waseda University

**Author(s) :** HRUSHIKESH N MHASKAR (Claremont Graduate University)

**Abstract :** We study the question of approximation of an operator  $\mathfrak{F}$  from one metric space  $X$  to another,  $Y$ . The input  $f \in X$  and  $\mathfrak{F}(f)$  are encoded in terms of a point on a sphere  $S^d$  ( $S^D$ ). Local approximation techniques are developed to achieve approximation of properly defined smooth function in a tractable manner.

## [04141] Neural operator surrogates for Gaussian inputs

**Format :** Talk at Waseda University

**Author(s) :** Jakob Zech (Universität Heidelberg)

**Abstract :** In this talk we discuss the use of operator surrogates to approximate smooth maps between infinite-dimensional Hilbert spaces. Such surrogates have a wide range of applications in uncertainty quantification and parameter estimation problems. The error is measured in the  $L^2$ -sense with respect to a Gaussian measure on the input space. Under suitable assumptions, we show that algebraic and dimension-independent convergence rates can be achieved.

## [03497] Derivative-Informed Neural Operators for Scalable and Efficient UQ

**Format :** Talk at Waseda University

**Author(s) :** Thomas O'Leary-Roseberry (The University of Texas at Austin)Omar Ghattas (The University of Texas at Austin)Peng Chen (Georgia Tech)Umberto Villa (The University of Texas at Austin)Dingcheng Luo (The University of Texas at Austin)Lianghao Cao (The University of Texas at Austin)

**Abstract :** We present a novel operator learning methodology "derivative-informed neural operators" (DINOs) that can accurately represent both operator maps and their derivatives in function spaces. DINOs are built using advanced adjoint methods and dimension reduction techniques, resulting in efficient computation of derivative quantities that can facilitate fast and scalable UQ. We showcase the potential of DINOs in two applications: Bayesian inversion using data from the 2011 Tōhoku earthquake, and optimal control of PDEs under uncertainty.

## [05169] Deep Operator Network Approximation Rates for Lipschitz Operators

**Format :** Online Talk on Zoom

**Author(s) :** Christoph Schwab (ETH Zurich)

**Abstract :** We establish expression rate bounds for neural Deep Operator Networks (DON) emulating Lipschitz continuous maps  $G$  between (suitable subsets of) separable Hilbert spaces  $X$  and  $Y$ . The DON architecture uses linear encoders  $E$  and decoders  $D$  via Riesz bases of  $X$ ,  $Y$ , and an approximator network of a parametric coordinate map that is Lipschitz continuous on the sequence space. The present results require mere Lipschitz (or Holder) continuity of  $G$ .

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00232 (3/3) : 2E @E704 [Chair: Samuel Lanthaler]

## [02675] Transfer Learning Enhanced Physics-informed DeepONets for Long-time Prediction

**Format :** Talk at Waseda University

**Author(s) :** wuzhe xu (University of Massachusetts Amherst)

**Abstract :** Deep operator network (DeepONet) has demonstrated great success in various learning tasks, including learning solution operators of partial differential equations. In particular, it provides an efficient approach to predict the evolution equations in a finite time horizon. Nevertheless, the vanilla DeepONet suffers from the issue of stability degradation in the long-time prediction. This paper proposes a transfer-learning aided DeepONet to enhance the stability. Our idea is to use transfer learning to sequentially update the DeepONets as the surrogates for propagators learned in different time frames. The evolving DeepONets can better track the varying complexities of the evolution equations, while only need to be updated by efficient training of a tiny fraction of the operator networks. Through systematic experiments, we show that the proposed method not only improves the long-time accuracy of DeepONet while maintaining similar computational cost but also substantially reduces the sample size of the training set.

## [03360] Generic bounds on the approximation error for physics-informed (and) operator learning

**Format :** Online Talk on Zoom

**Author(s) :** Tim De Ryck (ETH Zürich)Siddhartha Mishra (ETH Zürich)

**Abstract :** We propose a very general framework for deriving rigorous bounds on the approximation error for physics-informed neural networks (PINNs) and operator learning architectures such as DeepONets and FNOs as well as for physics-informed operator learning. These bounds guarantee that PINNs and (physics-informed) DeepONets or FNOs will efficiently approximate the underlying solution or solution operator of generic PDEs.

## [03124] Overcoming Fundamental Limitations of Current AI Approaches: From Digital to Analog Hardware

**Format :** Online Talk on Zoom

**Author(s) :** Gitta Kutyniok (LMU Munich)Holger Boche (TU Munich)Adalbert Fono (LMU Munich)Aras Bacho (LMU Munich)Yunseok Lee (LMU Munich)

**Abstract :** Artificial intelligence is currently leading to one breakthrough after the other. However, one current major drawback is the lack of reliability of such methodologies. In this talk, we will discuss fundamental limitations, showing that there do exist severe problems in terms of computability on any type of digital hardware, which seriously affects their reliability. At the same time, we also show that analog hardware such as neuromorphic computing or quantum computing could achieve true reliability.

## [00234] Differential Galois Theory and Integrability of Dynamical Systems

**Session Time & Room :**

00234 (1/2) : 2D (Aug.22, 15:30-17:10) @G404

00234 (2/2) : 2E (Aug.22, 17:40-19:20) @G404

**Type :** Proposal of Minisymposium

**Abstract :** The main objective of this minisymposium is to bring together researchers working on differential Galois theory and integrability of dynamical systems and to discuss recent results on the related topics containing the following:

- Developments of differential Galois theory in dynamical systems
- Integrability of dynamical Systems and PDE's
- Integrability in quantum mechanics and spectral theory
- Galois approach to nonintegrability

**Organizer(s)** : Kazuyuki Yagasaki

**Classification** : 34M15, 37J30, 12H05, 37J35, 37K10

**Minisymposium Program** :

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00234 (1/2) : 2D @G404 [Chair: Kazuyuki Yagasaki]

## [05314] The geodesic deviation equation for null geodesics in the Schwarzschild black-hole

**Format** : Talk at Waseda University

**Author(s)** : Juan José Morales-Ruiz (Universidad Politécnica de Madrid) Alvaro Pérez-Raposo (Universidad Politécnica de Madrid)

**Abstract** : The Schwarzschild black-hole is an integrable Hamiltonian system with four degrees of freedom. The geodesic deviation equations are the variational equations for this Hamiltonian system. By a joint theorem with Ramis, these equations can be solved in closed form in the framework of the differential Galois theory. This talk will be devoted to give the solutions of these equations around some null geodesics. This a joint work with Alvaro Pérez-Raposo.

## [03161] Non-integrability of a model of two tethered satellites

**Format** : Talk at Waseda University

**Author(s)** : Thierry Combot (Universite de Bourgogne)

**Abstract** : We study the integrability of a model of two tethered satellites whose centre of mass moves in a circular Keplerian orbit around a gravity centre. When tether rest length is zero, the model is integrable and even superintegrable for selected values of the parameters. For positive rest length, the system is non-integrable. Obstructions to integrability are obtained through study of the differential Galois group of an irreducible symplectic variational equation in dimension 4.

## [04393] Obstructions to integrability of nearly integrable dynamical systems

**Format** : Talk at Waseda University

**Author(s)** : Shoya Motonaga (Ritsumeikan University)

**Abstract** : We study necessary conditions for the existence of real-analytic first integrals and real-analytic integrability for perturbations of integrable systems including non-Hamiltonian ones in the sense of Bogoyavlenskij. Moreover, we compare our results with the classical results of Poincar'e and Kozlov for systems written in action and angle coordinates and discuss their relationships with the Melnikov methods for periodic perturbations of single-degree-of-freedom Hamiltonian systems. This is joint work with Kazuyuki Yagasaki at Kyoto University.

## [04873] A Tale of Two Polytopes related to geodesic flows on spheres

**Format** : Talk at Waseda University

**Author(s)** : Holger Rainer Dullin (University of Sydney) Diana Nguyen (University of Sydney) Sean Dawson (University of Sydney)

**Abstract** : Separation of variables for the geodesic flows on round spheres leads to a large family of integrable systems whose integrals are defined through the separation constants.

Reduction by the periodic geodesic flow leads to integrable systems on Grassmannians.

Specifically for the geodesic flow on the round  $S^3$  the reduced system defines a family of integrable systems on  $S^2 \times S^2$ . We show that the image of these systems under

a continuous momentum map defined through the action variables has a triangle as its image.

The image is rigid and does not change when the integrable system is changed within the family.

Each member of the family can be identified with a point inside a Stasheff polytope.

Corners of the polytope correspond to toric systems (possibly with degenerations),

edges correspond to semi-toric systems (in various meanings of the word),

and the face corresponds to "generic" integrable systems.

A fundamental difference of this momentum map to that of a toric or semi-toric system

is that the number of tori in the preimage of a non-critical point may be 1, 2, or 4.

The momentum map is continuous but not smooth along the images of hyperbolic singularities.

The corresponding quantum problem and generalisations to higher dimensional spheres will be discussed.

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00234 (2/2) : 2E @G404 [Chair: Juan Jose Morales-Ruiz]

**[03566] Local integrability and regularity of autonomous differential systems****Format :** Talk at Waseda University**Author(s) :** Xiang Zhang (Shanghai Jiao Tong University)

**Abstract :** For finite dimensional smooth autonomous differential systems, which have a singularity with one zero eigenvalue and the others nonresonant, we present our results on existence of local first integrals at the singularity, with emphasis on the regularity of the local first integrals. We first explore the existence of  $C^\infty$  local first integrals for analytic differential systems under the Poincaré's non-resonant condition. We then show that for the Gevrey class of vector fields, their local first integrals have the same regularity as that of the vector fields provided that the real parts of the nonresonant eigenvalues are all positive or all negative. Lastly, a sharper expression of the loss of the regularity is presented by the lowest order of the resonant terms together with the indices of Gevrey smoothness and the diophantine condition for the case that the Jacobian matrix of the vector field at the singularity is in the diagonal form. The main tools are the homological method, the KAM theory, and the Gevrey normalization theory.

**[04369] Singular solitary waves in the KdV equation****Format :** Talk at Waseda University**Author(s) :** Kazuyuki Yagasaki (Kyoto University)

**Abstract :** In this talk we consider the KdV equation and discuss its singular solitons which are called rational solitons, positons or negatons. We are especially interested in the solvability by quadrature for Schrödinger equations appearing as one of the related Lax pair. Some formulas for scattering coefficients of positons or negatons are also given. This is joint work with Katsuki Kobayashi.

**[04649] Korteweg-de Vries traveling waves and Differential Galois Theory****Format :** Online Talk on Zoom**Author(s) :** Maria-Angeles Zurro (Autonomous University of Madrid)

**Abstract :** It was conjectured that the abelianity of the identity component of the Galois group of the variational equation is a necessary condition for the integrability of the non-linear PDE itself. In my lecture I will present an algebraic and spectral study of the variational equation around a KdV solitonic potential from the point of view of Galois differential theory. This is part of an ongoing joint work with J. J. Morales-Ruiz and J.-P. Ramis.

**[03529] Real Liouvillian extensions of partial differential fields****Format :** Online Talk on Zoom**Author(s) :** Zbigniew Hajto (Faculty of Mathematics and Computer Science UJ)

**Abstract :** I will present Galois theory for partial differential systems defined over formally real differential fields with a real closed field of constants and over formally  $p$ -adic differential fields with a  $p$ -adically closed field of constants. For an integrable partial differential system, there exists a formally real (resp. formally  $p$ -adic) Picard-Vessiot extension. I will explain the applications of this theorem.

# [00237] Recent progress in multiscale modeling and computational methods in material sciences

**Session Time & Room :**

00237 (1/3) : 3D (Aug.23, 15:30-17:10) @G801

00237 (2/3) : 3E (Aug.23, 17:40-19:20) @G801

00237 (3/3) : 4C (Aug.24, 13:20-15:00) @G801

**Type :** Proposal of Minisymposium

**Abstract :** Remarkable progress has been made in recent years on multiscale modeling and computational methods for diverse problems in material sciences, including but not limited to fluid mechanics, pattern formation and defects in materials sciences, and soft and active materials in biology.

The research is interdisciplinary, spanning the fields of mathematics, materials science and biology. This minisymposium focuses on the recent progress in the multiscale modeling, mathematical analysis and computational methods of broad

topics in material sciences. We aim to bring together experts from diverse fields to share their interesting research topics and recent progress and to promote interdisciplinary research collaborations.

**Organizer(s)** : Chaozhen Wei, Dong Wang

**Classification** : 35Qxx, 74-xx, 76-xx, 65-xx, 49-xx, multiscale modeling, numerical methods, materials sciences

**Minisymposium Program** :

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00237 (1/3) : 3D @G801 [Chair: Chaozhen Wei]

## [05400] Numerical methods for topology optimization and applications

**Format** : Talk at Waseda University

**Author(s)** : Xiaoping Wang (Hong Kong university of science and technology)

**Abstract** : In this talk, I will introduce some numerical methods for topology optimization based on threshold dynamics method. Applications to linear elasticity, fluid network and porous media problems will be discussed.

## [05389] Optimal error estimate for the Multiscale Finite Element Method

**Format** : Talk at Waseda University

**Author(s)** : Pingbing Ming (Academy of Mathematics and Systems Science, Chinese Academy of Sciences) Siqi Song (Academy of Mathematics and Systems Science)

**Abstract** : We derive the optimal energy error estimate for multiscale finite element method with oversampling technique applying to elliptic systems with rapidly oscillating periodic coefficients that are bounded and measurable, which may admit rough microstructures. As a by-product of the energy estimate, we derive the rate of convergence in  $L^{d/(d-1)}$ -norm with  $d$  the dimensionality.

## [05618] On median filters for motion by mean curvature

**Format** : Talk at Waseda University

**Author(s)** : Selim Esedoglu (University of Michigan)

**Abstract** : The median filter scheme is an elegant, monotone discretization of the level set formulation of motion by mean curvature. It turns out to evolve every level set of the initial condition by another class of methods known as threshold dynamics. Based on this connection, we revisit median filters in light of recent work on the threshold dynamics method.

## [02920] Structure-preserving methods based on minimizing movement scheme for gradient flows with respect to transport distances

**Format** : Talk at Waseda University

**Author(s)** : Chaozhen Wei (University of Electronic Science and Technology of China)

**Abstract** : I will present a novel structure-preserving numerical method for gradient flows w.r.t Wasserstein-like transport distances induced by concentration-dependent mobilities, which arise widely in materials science and biology. Based upon the minimizing movement scheme and modern operator-splitting schemes, our method has built-in positivity or boundedness preserving, mass conservation, and energy-dissipative structures. I will show the flexibility and performance of our methods through simulation examples including different free energy functionals, general wetting boundary conditions and degenerate mobilities.

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00237 (2/3) : 3E @G801 [Chair: Dong Wang]

## [05350] Multi-scale modeling and simulations for two-phase flow with moving contact lines

**Format** : Talk at Waseda University

**Author(s)** : Xianmin Xu (Chinese Academy of Sciences)

**Abstract** : Two phase flow with moving contact lines is very difficult to model and simulate due to its multi-scale nature. The slipiness of the fluid molecules on solid substrates must be taken into account near the contact line in a continuum model since the standard no-slip boundary condition induces infinite energy dissipations. The microscopic roughness and inhomogeneity of the substrates make the problem even more challenging. In this talk, we will present some recent efforts to develop coarse-graining boundary condition and efficient numerical methods on the problem. In particular, we show that the Onsager principle can be used as an approximation tool to derive effective models for the dynamical multiscale problem.

### [04103] Energy stable methods for two-phase phase-field surfactant model

**Format :** Talk at Waseda University

**Author(s) :** Zhen Zhang (Southern University of Science and Technology)

**Abstract :** We develop energy stable and bound preserving schemes for phase-field surfactant model with moving contact lines. The desired properties of the schemes are rigorously proved. We numerically validate the accuracies of the schemes and apply them in simulating droplet impact problems. Qualitative agreements with experiments are obtained. Moreover, surfactants are observed to have effects on enhancing droplet deformation and reducing dissipations.

### [01396] Construction and Analysis for the Coupling Method of Atomistic and Higher Order Continuum Models

**Format :** Talk at Waseda University

**Author(s) :** Hao Wang (Sichuan University)Yangshuai Wang (University of British Columbia)

**Abstract :** Atomistic to continuum coupling methods have been widely used in the numerical simulation of crystal lattice with defects. In this talk, we present the construction and analysis of a coupling scheme that combines the atomistic model with a higher order continuum with sharp interface. We show that such scheme is of higher order of accuracy compared with existing models that couples the atomistic model with the classic Cauchy-Born model.

### [01316] A domain decomposition method for the Poisson-Boltzmann solvation model

**Format :** Talk at Waseda University

**Author(s) :** Chaoyu Quan (Southern University of Science and Technology)

**Abstract :** A nonoverlapping domain decomposition method is studied for the linearized Poisson--Boltzmann equation, which is essentially an interior-exterior transmission problem with bounded interior and unbounded exterior. This problem is different from the classical Schwarz alternating method for bounded nonoverlapping subdomains well studied by Lions in 1990, and is challenging due to the existence of unbounded subdomain. To obtain the convergence, a new concept of interior-exterior Sobolev constant is introduced and a spectral equivalence of related Dirichlet-to-Neumann operators is established afterwards. We prove rigorously that the spectral equivalence results in the convergence of interior-exterior iteration. Some numerical simulations are provided to investigate the optimal stepping parameter of iteration and to verify our convergence analysis.

00237 (3/3) : 4C @G801 [Chair: Chaozhen Wei]

### [01430] A Continuum Model for Dislocation Climb Velocity and Numerical Simulations

**Format :** Talk at Waseda University

**Author(s) :** Chutian Huang (Hong Kong University of Science and Technology)Yang Xiang (Hong Kong University of Science and Technology)

**Abstract :** Dislocations are primary carriers for the crystal plastic deformation. The study of dislocation climb plays an important role in understanding plastic deformation of crystalline deformation at high temperature. In this work, we propose a new continuum formulation for dislocation climb velocity. Numerical simulations are implemented to compare our model with mobility law and discrete model.

### [01298] A second-order in time, BGN-based PFEM for solving geometric PDEs

**Format :** Online Talk on Zoom

**Author(s) :** Wei Jiang (Wuhan University)Chunmei Su (Tsinghua University)Ganghui Zhang (Tsinghua University)

**Abstract :** We propose a higher-order in time, BGN-based parametric finite element method for solving geometric flows, e.g., curve shortening flow, area-preserving curve shortening flow and surface diffusion flow.

## [00239] Shape and Topology Optimizations

**Session Time & Room :**

00239 (1/2) : 5C (Aug.25, 13:20-15:00) @E710

00239 (2/2) : 5D (Aug.25, 15:30-17:10) @E710

**Type :** Proposal of Minisymposium

**Abstract :** Shape and topology optimizations are widely used in many industries and consider optimal shapes and topologies of materials to maximize desired physical properties. Topological changes also yield extremely high performance, and hence, these optimization methods have attracted much attention in many industries. Furthermore, recent technological innovations in additive manufacturing have made it possible to manufacture optimized materials and even metamaterials that do not exist in nature. Besides, these optimization methods that take manufacturability and practicality into consideration have also been developed and will be expected to be applied in various fields.

**Organizer(s) :** Takayuki Yamada, Grégoire Allaire, Hideyuki Azegami

**Classification :** 49-XX

**Minisymposium Program :**

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00239 (1/2) : 5C @E710 [Chair: Takayuki Yamada]

## [00244] PDEs for topology optimization considering manufacturability

**Format :** Talk at Waseda University

**Author(s) :** Takayuki Yamada (The University of Tokyo)

**Abstract :** The topology optimization framework is to have the PDEs of the physical field of interest as constraints. In this study, we propose PDEs that express target manufacturability in order to consider it in a topology optimization framework.

## [00368] Topology optimization of supports for additive manufacturing with accessibility constraints

**Format :** Talk at Waseda University

**Author(s) :** Grégoire Allaire (Ecole Polytechnique)Martin Bihr (Safran)Benjamin Bogosel (Ecole Polytechnique)

**Abstract :** This talk is concerned with an accessibility constraint, for shape and topology optimization of structures built by metallic additive manufacturing. Sacrificial supports are used to maintain a structure, during its building process. Removing them at the end is required but can be very difficult. Our work gives a new mathematical way to evaluate such an accessibility constraint, which is based on distance functions, solutions of eikonal equations. The main advantage is the possibility of computing shape derivatives of such a criterion with respect to both the structure and the support. We implement this accessibility constraint with the level-set method for topology optimization of structures.

## [03408] Dehomogenization in stress minimization problems

**Format :** Talk at Waseda University

**Author(s) :** Alex Ferrer (CIMNE)Grégoire Allaire (Ecole Polytechnique)Perle Geoffroy-Donders (Ecole Polytechnique)

**Abstract :** In the last years, additive manufacturing has allowed to build lattice structures with impressive small length scale. This breakthrough has forced the topology optimization community to propose fast multi-scale topology optimization techniques. The dehomogenization method has recently shown very promising results in terms of performance and computational cost for compliance examples. In this work, we extend it to stress minimization problems and by considering singularities in the orientation field.

## [03530] The topological ligament: an approach based on thin tubular inhomogeneities

**Format :** Talk at Waseda University

**Author(s) :** Charles Dapogny (CNRS & Université Grenoble Alpes)

**Abstract :** We propose a novel framework to calculate an approximate sensitivity of a functional depending on the domain with respect to the graft of a thin ligament. The resulting formulas are applied to:

- The addition of a thin ligament to a structure in the course of a classical shape optimization process;
  - The optimization of the scaffold structure of a 3d printed structure;
  - A "clever" initialization process for the optimization of a truss structure.
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00239 (2/2) : 5D @E710 [Chair: Takayuki Yamada]

## [00419] Level set-based topology optimization method with nonlinear diffusion

**Format :** Talk at Waseda University

**Author(s) :** Tomoyuki Oka (The University of Tokyo)Takayuki Yamada (The University of Tokyo)

**Abstract :** In this talk, we shall consider a level set-based topology optimization method with nonlinear diffusion.

Main results consist of the generalization of the method using reaction-diffusion equations, which improves convergence

part\_1

to optimized designs with the aid of singularity and degeneracy of diffusion coefficients, and therefore, a more practical method can be obtained.

## [00247] Interfaces and Free Boundaries in Fluid Mechanics and Materials Science

### **Session Time & Room :**

00247 (1/2) : 3E (Aug.23, 17:40-19:20) @G710

00247 (2/2) : 4C (Aug.24, 13:20-15:00) @G710

**Type :** Proposal of Minisymposium

**Abstract :** This minisymposium is focused on recent advances in the analysis of interface evolution problems. A particular emphasis lies on prominent applications arising in materials science (grain coarsening in polycrystalline materials), fluid mechanics (fluid-structure interaction, viscous surface waves, dynamic wetting) and phase separation models from chemistry. The minisymposium brings together an international group of researchers, new and established, to discuss topics covering a broad range of associated mathematical questions and techniques. These include variational methods for modelling and solution theories, the rigorous derivation of sharp interface limits, and the analysis of evolving networks of branched interfaces.

**Organizer(s) :** Sebastian Hensel, Kerrek Stinson

**Classification :** 35R35, 35A15, 74N20

### **Minisymposium Program :**

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00247 (1/2) : 3E @G710 [Chair: Kerrek Stinson]

## [02095] On the notion of generalized mean curvature flow

**Format :** Talk at Waseda University

**Author(s) :** Yoshihiro Tonegawa (Tokyo Institute of Technology)

**Abstract :** I describe some new aspects of generalized notion of mean curvature flow which are prompted by various attempts to prove the existence, uniqueness and regularity. The main tool comes from geometric measure theory which allows treatments of singular geometric objects necessary to deal with the weak formulation of mean curvature flow.

## [03166] Coarsening phenomena in the network flow

**Format :** Talk at Waseda University

**Author(s) :** Alessandra Pluda (University of Pisa)

**Abstract :** A network is a 1-dimensional connected set in the plane composed of a finite number of curves that meet at their endpoints in junctions. The flow by curvature of networks has been introduced in mathematical materials science to model the evolution of polycrystals. We would like to formalise a coarsening behavior, suggested by numerical simulations. I will present the mathematical tools developed to describe this evolution and an argument which supports the coarsening behavior.

## [03048] Uniqueness and stability of multiphase mean curvature flow beyond a singular time: the case of the shrinking circle

**Format :** Talk at Waseda University

**Author(s) :** Alice Marveggio (Institute of Science and Technology Austria (ISTA)) Julian Fischer (Institute of Science and Technology Austria (ISTA)) Maximilian Moser (Institute of Science and Technology Austria (ISTA)) Sebastian Hensel (Hausdorff Center for Mathematics, University of Bonn)

**Abstract :** The evolution of a network of interfaces by mean curvature flow features the occurrence of topology changes and geometric singularities. As a consequence, classical solution concepts for mean curvature flow are in general limited to short-time existence theorems, which include singular times only for some stable shrinkers such as the circle. At the same time, the transition from strong to weak solution concepts (e.g. Brakke solutions) may lead to non-uniqueness of solutions.

Following the relative energy approach à la Fischer-Hensel-Laux-Simon and introducing a suitable notion of gradient-flow calibration for a shrinking circle, we prove a quantitative stability estimate holding up to the singular time. This implies a weak-strong uniqueness principle for weak BV solutions to planar multiphase mean curvature flow beyond a

specific class of singularities.

Furthermore, we expect our method to have further applications to other types of shrinkers, as well as to prove quantitative convergence of diffuse-interface (Allen-Cahn) approximations for mean curvature flow.

## [02872] Matrix-valued Allen–Cahn equation and the Keller–Rubinstein–Sternberg problem

**Format :** Talk at Waseda University

**Author(s) :** Mingwen Fei Fanghua Lin (Courant Institute of Mathematical Science, New York University)Wei Wang (Zhejiang University)Zhifei Zhang (Peking University)

**Abstract :** In this talk, we consider the sharp interface limit of a matrix-valued Allen-Cahn equation. We show that the sharp interface system is a two-phases flow system: the interface evolves according to the motion by mean curvature; in the two bulk phase regions, the solution obeys the heat flow of harmonic maps with values in  $n \times n$  orthogonal matrices with determinant +1 and -1 respectively; on the interface, the phase matrices in two sides satisfy a novel mixed boundary condition. The above result provides a solution to the Keller-Rubinstein-Sternberg's problem in the  $O(n)$  setting. Our proof relies on two key ingredients. First, in order to construct the approximate solutions by matched asymptotic expansions, as the standard approach does not seem to work, we introduce the notion of quasi-minimal connecting orbits. They satisfy the usual leading order equations up to some small higher order terms. In addition, the linearized systems around these quasi-minimal orbits needs to be solvable up to some good remainders. These flexibilities are needed for the possible "degenerations" and higher dimensional kernels for the linearized operators on matrix-valued functions due to intriguing boundary conditions at the sharp interface. The second key point is to establish a spectral uniform lower bound estimate for the linearized operator around approximate solutions. To this end, we introduce additional decompositions to reduce the problem into the coercive estimates of several linearized operators for scalar functions and some singular product estimates which are accomplished by exploring special cancellation structures between eigenfunctions of these linearized operators.

00247 (2/2) : 4C @G710 [Chair: Alessandra Pluda]

## [03054] Variational methods for time-dependent problems on dynamically changing domains

**Format :** Talk at Waseda University

**Author(s) :** Malte Kampschulte (Charles University Prague)

**Abstract :** In this talk I will present a general, energetically consistent method that can be used to show the existence of weak solutions for nonlinear problems in fluid structure-interaction and related fields. Not only can this be done without the need to make simplifying assumptions on domain or equations, in fact it crucially relies on all physical terms being present. This talk is based on several recent results primarily with B.Benesova, S.Schwarzacher but also D.Breit, A.Cesik, G.Gravina and G.Sperone.

## [04468] Sharp-interface limit of models with mechanics and contact lines

**Format :** Talk at Waseda University

**Author(s) :** Dirk Peschka (WIAS Berlin & Freie Universität Berlin)Leonie Schmeller (Weierstrass Institute)

**Abstract :** First, we construct gradient structures for free boundary problems including nonlinear elasticity, phase fields and moving contact lines, where the convergence of phase-field models to certain sharp-interface limits is analyzed numerically. Then, in the second part of the talk, it will be shown how shapes of droplets on soft elastic substrates can be predicted by corresponding (sharp-interface) models, and some emergent phenomena - cloaking and phase separation near the contact line - are pointed out.

## [03766] Uniform Rectifiability for Minimizers of the Griffith Fracture Energy

**Format :** Talk at Waseda University

**Author(s) :** Kerrek Stinson (University of Bonn)Manuel Friedrich (University of Erlangen-Nuremberg)Camille Labourie (University of Erlangen-Nuremberg)

**Abstract :** Recent studies for minimizers of the Griffith energy, which penalizes elastic energy and fracture, have relied on topological constraints for the (codimension-1) crack. Regularity results effectively say that if the crack locally separates the domain into different connected components, then the crack is in fact a smooth surface. Our analysis looks at minimizers without topological constraints. As a first step, we prove uniform rectifiability, which shows that on sufficiently small scales, the crack is nearly topologically separating. The purpose of this talk is to illuminate the new techniques applied in this setting and discuss how a similar approach can be used to prove a regularity result for the crack.

# [00253] Modelling and Simulation of Lithium-Ion Batteries

## **Session Time & Room :**

00253 (1/3) : 4C (Aug.24, 13:20-15:00) @D403

00253 (2/3) : 4D (Aug.24, 15:30-17:10) @D403

00253 (3/3) : 4E (Aug.24, 17:40-19:20) @D403

## **Type :** Proposal of Minisymposium

**Abstract :** Lithium-ion batteries have a very important role to play in the transition to a sustainable future. But despite the current widespread use of batteries, many of the phenomena involved in their functioning are not well understood. Mathematical models can be a fundamental tool to understand batteries and enable better design and management. In this minisymposium we will discuss the latest advances in the development and analysis of continuum models for lithium-ion batteries, with a particular focus on homogenised models and their applications to real-world problems. This minisymposium is part of the ECMI Special Interest Group on Sustainable Energies and Materials.

## **Organizer(s) :** Ferran Brosa Planella

**Classification :** 76Rxx, 76Sxx, 76Txx, 80Axx, 92Exx

## **Minisymposium Program :**

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00253 (1/3) : 4C @D403 [Chair: Ferran Brosa Planella]

## [03631] Asymptotic methods for lithium-ion battery models

### **Format :** Talk at Waseda University

### **Author(s) :** Ferran Brosa Planella (University of Warwick)

**Abstract :** Lithium-ion batteries have become an essential in our lives, and to develop better and safer batteries we need accurate and fast models. Current models are often posed in an ad hoc way, which usually leads to inconsistencies. In this talk we will provide an overview of battery modelling, and show how asymptotic methods can help us obtain simple and consistent models that help us design and manage the next generation of batteries.

## [05237] Topology Optimization for Li-ion batteries

### **Format :** Talk at Waseda University

**Author(s) :** Thomas Roy (Lawrence Livermore National Laboratory)Hanyu Li (Lawrence Livermore National Laboratory)Nicholas Brady (Lawrence Livermore National Laboratory)Giovanna Bucci (Lawrence Livermore National Laboratory)Tiras Lin (Lawrence Livermore National Laboratory)Daniel Tortorelli (Lawrence Livermore National Laboratory)Marcus Worsley (Lawrence Livermore National Laboratory)

**Abstract :** Typical porous electrodes are homogeneous, stochastic collections of small-scale particles offering few opportunities for engineering higher performance. To leverage recent breakthroughs in advanced and additive manufacturing, we use topology optimization to design electrodes for energy storage devices. Energy density is maximized, leading to non-trivial geometries that outperform monolithic electrodes. These geometries facilitate ionic transport and lead to better electrode utilization. We consider simultaneous optimization of cathode and anode, which can lead to interdigitated designs. LLNL-ABS-847750

## [04263] Homogenisation and Modelling of a Silicon nanowire Li-ion battery anode

### **Format :** Talk at Waseda University

**Author(s) :** Emma Elizabeth Greenbank (MACSI, University of Limerick)Michael Vynnycky (MACSI, University of Limerick)Doireann O'Kiely (MACSI, University of Limerick)

**Abstract :** We consider a battery anode composed of an array of copper nanowires, coated with Li-carrying copper silicide and surrounded by Li-alloying electrolyte. This anode design alleviates degradation arising from extreme volumetric changes of silicon during lithiation. The governing equations for the electric and concentration fields inside the nanowire array structure are homogenised, and solutions of the homogenised problem are used to predict the transport of lithium through the anode.

## [02731] A continuum model for lithium plating and dendrite formation in lithium-ion batteries.

**Format :** Talk at Waseda University

**Author(s) :** Smita Sahu (University of Portsmouth)

**Abstract :** This work presents a novel physics-based model for lithium plating and dendrite formation in lithium-ion batteries. The formation of Li metal is an undesirable side-effect of fast charging and a primary contributor to cell degradation and failure. The model distinguishes between three types of plated Li metal, namely: (a) Li metal plated within the pores of the solid electrolyte interphase (assumed to be electronically connected to the anode and therefore recoverable); (b) dendrites protruding outside the SEI that remain electronically connected (and are therefore dangerous, potentially leading to a short circuit), and (c) electronically disconnected/“dead” Li metal outside the SEI contributing to capacity fade. The model is validated against two independent experiments. First, measurements of: (i) the cell voltage and current during a constant-current-constant-voltage charge and subsequent discharge, and (ii) the Li metal intensities (derived from operando NMR) which directly quantifies the time-resolved quantity of Li metal in the cell during use. Second, against voltage measurements during galvanostatic discharge at a range of C-rates and temperatures. Favourable agreement is demonstrated throughout; particularly in terms of the proportions of reversible and irreversible plating. We also demonstrate that the model reproduces the well-documented trends of being more prevalent at increased C-rate and/or decreased temperature.

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00253 (2/3) : 4D @D403 [Chair: Ferran Brosa Planella]

## [04505] Simulation and analysis of space charge layers in a solid electrolyte

**Format :** Talk at Waseda University

**Author(s) :** Laura Marie Keane (York University)Iain Moyles (York University)

**Abstract :** We consider the zero-charge flux equilibrium problem in a solid electrolyte. We introduce an auxiliary variable to remove singularities from the domain, facilitating robust numerical simulations. We use asymptotic reduction to uncover the true width of the boundary layer of the electrolyte. Exploiting the asymptotic regimes, we generate a nonuniform discretization grid enabling more computationally efficient simulations without sacrificing accuracy as we focus computational power in regions where the solution changes more rapidly.

## [03112] Machine Learning of Electrochemistry Battery Models

**Format :** Talk at Waseda University

**Author(s) :** Brian Wetton (University of British Columbia)Maricela Best-Mckay (University of British Columbia)

**Abstract :** We present a surrogate modeling approach that uses synthetic data generated by an electrochemical model to approximate Li-ion battery dynamics using a Deep Neural Network. Our approach uses the Pseudo-Two Dimensional model and a well defined use-cycle, fit to a Network of convolution type for the particle concentrations. The Network is able to accurately predict future behaviour. Extensions to initial State of Charge correction and the identification of a State of Health parameter are given.

## [05150] Parameterisation of reduced-order battery models from non-invasive characterisation

**Format :** Talk at Waseda University

**Author(s) :** Nicola Courtier (University of Oxford)Ross Drummond (University of Sheffield)David Howey (University of Oxford)

**Abstract :** Robust parameterisation methods exist for equivalent circuit models of batteries but, to understand the underlying processes and battery design, electrochemical models are needed. Progress is limited by a lack of robust parameterisation methods for nonlinear systems of differential equations, containing parameters which are unidentifiable from non-invasive measurements. Reduced-order modelling offers a pathway to systematically estimate lumped parameters from data using prediction-error minimisation. Furthermore, we apply the measure-moment approach to optimisation to estimate optimal charging profiles.

## [05185] Early prediction of battery remaining useful life using AI and physics

**Format :** Online Talk on Zoom

**Author(s) :** Edwin Khoo (Institute for Infocomm Research (I2R), Agency for Science, Technology and Research (A\*STAR))

**Abstract :** Accurate prediction of the remaining useful life (RUL) of a lithium-ion battery (LIB) using early cycle data aids in scheduling predictive maintenance, avoiding catastrophic failure during operation and optimizing battery manufacturing. In this talk, we discuss our recent work in building a hybrid deep learning model that combines physics-informed features with statistical features to achieve better generalization performance in early RUL prediction when

benchmarked against several AI models. If time permits, we will also discuss our recent parametric study of LIB capacity fade using a cell OCV model.

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00253 (3/3) : 4E @D403

## [00255] Recent developments in fast algorithms for inverse problems and imaging

### **Session Time & Room :**

00255 (1/2) : 3D (Aug.23, 15:30-17:10) @E819

00255 (2/2) : 3E (Aug.23, 17:40-19:20) @E819

**Type :** Proposal of Minisymposium

**Abstract :** Inverse problems correspond to the reconstruction of hidden objects from possibly noisy indirect measurements and are ubiquitous in a variety of scientific and engineering applications. Since these problems tend to be ill-posed, and real-world applications are often large-scale, this can be a very challenging task. This minisymposium focuses on recent advances in computationally efficient methods for solving large-scale inverse problems in imaging, e.g., those arising in medical, geophysical and industrial applications, covering topics that include advances in iterative methods, regularization, machine learning and novel applications of the previous.

**Organizer(s) :** Malena Sabaté Landman, Jiahua Jiang

**Classification :** 68U10, 65F22, 65F10, 15A29

### **Minisymposium Program :**

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00255 (1/2) : 3D @E819 [Chair: Malena Sabaté Landman]

## [03339] Streaming Methods for Inverse Problems

**Format :** Talk at Waseda University

**Author(s) :** Eric de Sturler (Virginia Tech)

**Abstract :** We discuss Golub-Kahan type methods for streaming problems. As big data applications become ever more prominent, in many applications we can only solve problems such as linear or nonlinear regression problems in chunks. Data may come in over a larger span of time and we cannot (or prefer not) to wait until all data is available, the problem may be too large to fit in memory, or data is coming in at a rate that we can use only sampled data and use it in chunks. There is a need for methods that can work efficiently under such conditions. We discuss extensions for GKB-type methods that select and build effective search spaces over multiple subsets of data and/or matrix-blocks to compute accurate solutions with limited memory available. Apart from streaming applications this may also be useful for modern computing architectures that have highly non-uniform memory access.

This is joint work with Julianne Chung, Jiahua Jiang, Misha Kilmer, and Mirjeta Pasha.

## [03433] Sequential model correction for nonlinear inverse problems

**Format :** Talk at Waseda University

**Author(s) :** Arttu Arjas (University of Oulu)Andreas Hauptmann (University of Oulu)Mikko Sillanpää (University of Oulu)

**Abstract :** Linear inverse problems are usually solved with first-order gradient methods. For nonlinear problems one must resort to second-order methods that are computationally more expensive. In this work we approximate a nonlinear model with a linear one and correct the resulting approximation error. We develop a sequential method that iteratively solves a linear inverse problem and updates the approximation error. We analyze the sequence theoretically and present numerical results.

## [02062] Plants, robots and dynamic tomography

**Format :** Talk at Waseda University

**Author(s) :** Tommi Heikkilä (University of Helsinki)

**Abstract :** The need for dynamic tomography can arise from many applications, e.g. imaging nutrient perfusion in plant stems for carbon uptake and metabolism studies. While the measurements may be sparse, obtaining the reconstructions can be computationally intensive, since 3D volumes evolving over time leads to 4D tomography. Thus we need fast and efficient methods: our choice are sparse representation systems such as (complex) wavelets and (cylindrical) shearlets, tested on dynamic data from a motorized phantom.

**[04602] Deep learning methods for data-driven uncertainty quantification****Format** : Talk at Waseda University**Author(s)** : Ling Guo (Shanghai Normal University )**Abstract** : In this talk, we will present some recent developments on using Physics-informed neural networks (PINNs) to quantify uncertainty propagation in a unified framework forward, inverse and mixed stochastic problems based on scattered measurements. We will also present generative models for data-driven uncertainty quantification, including physics-informed generative adversarial networks and Normalizing field flows.

00255 (2/2) : 3E @E819 [Chair: Malena Sabaté Landman]

**[04412] Exploiting Mixed Precision Arithmetic in Image Reconstruction****Format** : Talk at Waseda University**Author(s)** : James Nagy (Emory University)**Abstract** : Although some work has been done to exploit mixed precision computations for inverse problems arising in image processing, most previous work focuses on extended precision to avoid the influence of rounding errors. We consider a different perspective: because we cannot expect to precisely know data, we develop and analyze solvers that can take advantage of low precision speed of modern computer architectures, and which can be used in a variety of imaging applications.**[03595] Image Quality Assessment for Reconstruction Algorithms****Format** : Talk at Waseda University**Author(s)** : Anna Breger (University of Cambridge)**Abstract** : Assessing digital image quality (IQ) is of high importance in numerous applied research fields, such as image acquisition, reconstruction or processing. Automated evaluation is needed since manual evaluation is too time-consuming and expensive for huge data sets and, furthermore, may be biased or introduce inconsistencies. In this talk I will give a short introduction to IQ assessment and provide examples of failure when applying standard full reference IQ measures in medical imaging reconstruction tasks.**[00260] Statistics for random dynamics****Session Time & Room** : 1C (Aug.21, 13:20-15:00) @E504**Type** : Proposal of Minisymposium**Abstract** : Nowadays, a broad spectrum of large-scale and high-frequency data sets with complex spatiotemporal dependent structures is available; relevant fields of research are wide-ranging, including biology, finance, and actuarial science, to mention just a few. To create white-box models equipped with efficient and practical mechanisms for such data sets, simple combinations of the currently available devices are not enough, and it is therefore urgent and imperative to develop both mathematical statistics for stochastic processes and stochastic analyses synergistically, learning new from the past. Our session is intended to present some state-of-the-art topics in this active area of research.**Organizer(s)** : Hiroki Masuda, Shiochi Eguchi**Classification** : 62Mxx, 60Fxx, 60Gxx, 60Hxx**Minisymposium Program** :

00260 (1/1) : 1C @E504 [Chair: Hiroki Masuda]

**[03955] Online parametric estimation of stochastic differential equations with discrete observations****Format** : Talk at Waseda University**Author(s)** : Shogo Nakakita (University of Tokyo)**Abstract** : We consider online parametric estimation for stochastic differential equations based on discrete observations. The proposed method uses an online gradient descent method for negative quasi-log-likelihood functions with convexity and achieves low computational complexity. We derive a non-asymptotic uniform upper bound for the risk of the estimation by our results on stochastic optimization and ergodicity.

## [03956] Weighted block bootstrap for misspecified ergodic Lévy driven SDE models

**Format :** Talk at Waseda University

**Author(s) :** Yuma Uehara (Kansai University)

**Abstract :** In this talk, we consider possibly misspecified stochastic differential equation models driven by L'levy processes. Under some regularity conditions, Gaussian quasi-likelihood estimator can estimate unknown parameters in the drift and scale coefficients. However, especially in the misspecified case, it is hard to construct a consistent estimator of the asymptotic variance directly. For such a problem, we propose a weighted block bootstrap procedure to evaluate the asymptotic distribution.

## [04399] Robustifying Gaussian quasi-likelihood inference for random dynamics

**Format :** Talk at Waseda University

**Author(s) :** Shoichi Eguchi (Osaka Institute of Technology)

**Abstract :** We consider Gaussian quasi-likelihood inference for stochastic differential equations. In this study, suppose that the observations are obtained from the L'levy process with the compound-Poisson jumps and spike noises, and we regard jumps and spike noises as outliers that disturb the parameter estimation. We construct an estimator without reference to the presence of the jump component and some spike noises, in addition to that of the drift term.

## [04695] Asymptotic expansion of estimator of Hurst parameter of SDE driven by fractional Brownian motion

**Format :** Talk at Waseda University

**Author(s) :** Hayate Yamagishi (University of Tokyo)

**Abstract :** Asymptotic expansion is presented for an estimator of the Hurst coefficient of a stochastic differential equation driven by a fractional Brownian motion of  $H>1/2$ . While applying a recently developed theory of asymptotic expansion of Wiener functionals to the estimator, the main difficulty is to estimate orders of complicated functionals appearing in expanding the estimator and identifying the limit random symbols. To overcome the difficulty, we introduce a theory of an exponent based on weighted graphs.

# [00262] numerical analysis, modeling and applications in phase-field its relevant methods

**Session Time & Room :**

00262 (1/3) : 3C (Aug.23, 13:20-15:00) @E705

00262 (2/3) : 3D (Aug.23, 15:30-17:10) @E705

00262 (3/3) : 3E (Aug.23, 17:40-19:20) @E705

**Type :** Proposal of Minisymposium

**Abstract :** The phase field method and its relevant extensions have been widely used in various applications, including phase separations, crystal growth, and solid fracture dynamics. Meanwhile, it is still an active research field to develop thermodynamically consistent phase field models, design accurate, efficient, and stable numerical algorithms for these models, and apply them to various application problems. This mini-symposia brings together experts with diverse backgrounds in numerical analysis, PDE modeling and mathematical biology, machine learning, and data science, but with the same interest in phase field method and its relevant extension. Through this mini-symposia, we aim to foster active interdisciplinary discussions.

**Organizer(s) :** Xiaofeng Yang; Xiaoming He; Jia Zhao

**Classification :** 65Mxx, 65Nxx, 65Zxx

**Minisymposium Program :**

00262 (1/3) : 3C @E705 [Chair: Xiaofeng Yang]

## [05280] Approximating Structurally Unstable Over-determined Systems of PDEs

**Author(s)** : Qi Wang (University of South Carolina)

**Abstract** : Models for nonequilibrium phenomena are normally consisted of differential equations, from which some physically important relations can be deduced. Together, they form an extended, over-determined system of equations which is normally structurally unstable. Structure-preserving approximation thus ensues, which are known numerically as structure-preserving algorithms/schemes. In this presentation, I will discuss some structure-preserving numerical strategies for developing numerical algorithms for thermodynamically consistent multiphase materials models, which are derived from thermodynamical principles.

## [03012] Energy stability analysis and error estimate of a maximum bound principle preserving scheme for the dynamic Ginzburg--Landau equations under the temporal gauge

**Author(s)** : Zhonghua Qiao (The Hong Kong Polytechnic University)

**Abstract** : This paper proposes a decoupled numerical scheme of the time-dependent Ginzburg--Landau equations under the temporal gauge. For the magnetic potential and the order parameter, the discrete scheme adopts the second type Nedélec element and the linear element for spatial discretization, respectively; and a linearized backward Euler method and the first order exponential time differencing method for time discretization, respectively. The maximum bound principle (MBP) of the order parameter and the energy dissipation law in the discrete sense are proved. The discrete energy stability and MBP-preservation can guarantee the stability and validity of the numerical simulations, and further facilitate the adoption of adaptive time-stepping strategy, which often plays an important role in long-time simulations of vortex dynamics, especially when the applied magnetic field is strong. An optimal error estimate of the proposed scheme is also given. Numerical examples verify the theoretical results of the proposed scheme and demonstrate the vortex motions of superconductors in an external magnetic field.

## [04941] Phase-field modelling of three-phase solidification with density variation

**Author(s)** : Pengtao Yue (Virginia Tech)Jiaqi Zhang (Beijing Normal University-Hong Kong Baptist University United International College)Yichen Li (Virginia Tech)

**Abstract** : We present a non-isothermal quasi-incompressible phase-field model for three-phase solidification that involves water, ice, and air. Water-ice phase transition and water-air interface are handled by the Allen-Cahn and Cahn-Hilliard equations, respectively. Constitutive relations are derived based on non-negative entropy production. Our model automatically captures curvature and pressure effects as dictated by the Gibbs-Thomson and Clausius-Clapeyron equations, as well as volume expansion during solidification. Numerical results on tip formation of a freezing droplet will be presented.

## [02938] Multiscale topology optimization method for lattice materials

**Author(s)** : Yibao Li (Xi'an Jiaotong University)Qing Xia (Xi'an Jiaotong University)Xin Song (Xi'an Jiaotong University)Qian Yu (Xi'an Jiaotong University)Binhu Xia (Xijing University )

**Abstract** : In this talk, we will introduce an efficient multiscale topology optimization method for lattice materials. In macro-scale, we present a second-order unconditionally energy stable schemes for the topology optimization problem. Using porous media approach, our objective functional composes of five terms including mechanical property, Ginzburg-Landau energy, two penalized terms for solid and the volume constraint. A Crank-Nicolson method is proposed to discrete the coupling system. We prove that our proposed scheme is unconditionally energy stable. In macro-scale, we propose a simple volume merging method for triply periodic minimal structure. A modified Allen-Cahn type equation with a correction term is proposed. The mean curvature on the surface will be constant everywhere at the equilibrium state. Computational experiments are presented to demonstrate the efficiency of the proposed method.

00262 (2/3) : 3D @E705 [Chair: Xiaoming He]

## [04079] New unconditionally stable higher-order consistent splitting schemes for the Navier-Stokes equations

**Author(s)** : JIE SHEN (Purdue University)Fukeng Huang (National University of Singapore)

**Abstract** : The consistent splitting schemes for the Navier-Stokes equations decouple the computation of pressure and velocity, and do not suffer from the splitting error. However, only the first-order version of the consistent splitting schemes is proven to be unconditionally stable for the time dependent Stokes equations.

We construct a new class of consistent splitting schemes of orders two to four for Navier-Stokes equations based on Taylor expansions at time  $t_{n+k}$  where  $k \geq 1$  is a tunable parameter. We show that, for some suitable choices of  $k$ , they are unconditionally stable for the time dependent Stokes equations, and by combining them with the generalized scalar auxiliary variable (GSAV) approach, we construct, for the very first time, unconditionally stable (in  $H^1$  norm) and totally decoupled schemes of orders two to four for the velocity and pressure, and provide rigorous optimal error estimates. We shall also present some numerical results to show the computational advantages of these schemes.

## [04302] Multi-phase-field modeling of grain growth and multiphase flow in additive manufacturing

**Author(s)** : Tomohiro Takaki (Kyoto Institute of Technology)

**Abstract** : A multi-phase-field model for predicting material microstructures formed during the powder bed fusion additive manufacturing of a metallic alloy is developed. Here, multi-phase-field models for solidification and multiphase flow problems are coupled to express polycrystalline solidification with melt flow in the melt pool.

## [04437] An efficient nonsmooth global optimization-based bound-preserving approach for the Cahn-Hilliard equation

**Author(s)** : Xiangxiong Zhang (Purdue University)

**Abstract** : It is quite difficult to construct bound-preserving schemes for many high order time-dependent PDEs. For instance, it is difficult to prove that the Cahn-Hilliard equation with polynomial potential admits a bound-preserving solution, yet a bound-preserving numerical solution is often preferred. Instead of directly constructing a bound-preserving scheme, we consider a global optimization based post processing in each time. Due to the nonsmooth terms in the cost function, such an optimization based approach has often been regarded as inefficient. However, it is possible to obtain an efficient solver by using optimal parameters obtained from asymptotic convergence rate formula. We demonstrate that the selection of optimization algorithm parameters from combining such an asymptotic convergence rate formula with time continuation in a time-dependent problem can give an efficient high order accurate bound-preserving post-processing solver, which costs  $O(n)$  per time step.

## [05375] Efficient decoupling energy stable approach for coupled type gradient flow systems with anisotropy for alloys

**Author(s)** : Xiaofeng Yang (University of South Carolina)

**Abstract** : The multi-component alloy phase-field model is a highly complex coupled gradient-like flow model that involves the coupling of multiple Allen-Cahn/Cahn-Hilliard equations with different types of flow field equations. Our ultimate goal is to develop efficient numerical algorithms of the decoupling type for this model. In our initial attempt, we focus on designing a second-order linear unconditional energy stable scheme for the solidification of pure metal, which is further coupled with free flow incorporating Darcy's force. The numerical method is primarily based on the derivative class of the IEQ (Invariant Energy Quadratization) method, which has gained prominence in recent years. Specifically, we combine the so-called EIEQ method with the modified projection method and employ the novel ZEC (Zero-Energy-Contribution) decoupling method to obtain the desired numerical scheme. This approach is versatile and can be applied to a wide range of models involving flow, magnetic, and electric field coupling. To validate the effectiveness of the scheme, we conduct extensive 2D and 3D numerical simulations as well.

00262 (3/3) : 3E @E705 [Chair: Jia Zhao]

## [03552] High-order exponential integrators for semilinear parabolic equations with nonsmooth data

**Author(s)** : Shu MA (City University of Hong Kong)Buyang Li (The Hong Kong Polytechnic University)

**Abstract** : A multistep exponential integrator is proposed for the semilinear parabolic equation with nonsmooth initial data, using variable stepsizes and contour integral approximations to address the initial singularity. The approach is extended to the semilinear subdiffusion equation with nonsmooth initial data. We propose an exponential convolution quadrature that combines contour integral representation of the solution, quadrature approximation of contour integrals, multistep exponential integrators for ordinary differential equations, and locally refined stepsizes to resolve the initial singularity. The proposed  $k$ -step exponential integrator and exponential convolution quadrature can have  $k$ th-order convergence for bounded measurable solutions of the semilinear parabolic and subdiffusion equations, respectively, based on the natural regularity of the solutions corresponding to the bounded measurable initial data.

## [04765] Mathematical modeling and numerical approximation of bulk-surface model

**Author(s)** : Xueping Zhao (University of Nottingham Ningbo China)

**Abstract** : In biological systems, many molecules, such as proteins and RNAs can phase separate and form liquid condensates in living cells. Many of those biological molecules can bind to the biological surfaces with some domains. How the kinetic processes are affected by surface binding is still unknown. Here, we derive the governing equations of the bulk-membrane coupled system with membrane-binding using irreversible thermodynamic theory. A three-dimensional numerical solver for kinetic equations is developed to study the effects of membrane binding on the various kinetic process. Our results suggest that membrane binding play crucial roles in the underlying physical principles(e.g. time scales) of kinetic processes of the bulk-membrane system.

## [02279] Discovery of Governing Equations with Recursive Deep Neural Networks

**Author(s)** : Jia Zhao (Utah State University)

**Abstract** : In this talk, I will focus on the model discovery problem when the data is not efficiently sampled. This is common due to limited experimental accessibility and labor/resource constraints. Specifically, we introduce a recursive deep neural network (RDNN) for data-driven model discovery. By embedding the known physics knowledge, this recursive approach can retrieve the governing equation in a simple and efficient manner, and it can significantly improve the approximation accuracy by increasing the recursive stages.

# [00263] Problems in incompressible fluid flows: Stability, Singularity, and Extreme Behavior

**Session Time & Room :**

00263 (1/3) : 1C (Aug.21, 13:20-15:00) @D401

00263 (2/3) : 1D (Aug.21, 15:30-17:10) @D401

00263 (3/3) : 1E (Aug.21, 17:40-19:20) @D401

**Type** : Proposal of Minisymposium

**Abstract** : The objective of the mini-symposium is to survey recent progress regarding a number of problems in theoretical fluid mechanics and to foster an exchange of new ideas in this field. It will cover a range of topics related to the existence of equilibrium solutions and their stability, extreme behaviors realizable in fluid flows, regularity of solutions versus singularity formation, transport, and turbulence. Both vicious and inviscid flows will be considered as well as some other simplified models of fluid flow. The mini-symposium will emphasize insights obtained by exploiting connections between rigorous mathematical analysis, physics, and numerical computations.

**Organizer(s)** : Takashi Sakajo, Bartosz Protas

**Classification** : 76D05, 35Q30, 35Q31, 76F02, 35A21

**Minisymposium Program :**

00263 (1/3) : 1C @D401 [Chair: Bartosz Protas]

## [00695] Enforcing conservation laws in truncated fluid models: the effect on heavy-tailed statistics

**Format** : Online Talk on Zoom

**Author(s)** : Mohammad Farazmand (North Carolina State University)Zack Hilliard (North Carolina State University)

**Abstract** : A significant class of partial differential equations (PDEs) have conserved quantities, arising from conservation of mass, energy, momentum, etc. These conserved quantities are not necessarily preserved when the PDE is discretized for numerical simulations. A recent method called reduced-order nonlinear solutions (RONS) allows us to ensure these conserved quantities are preserved after a Galerkin-type truncation of the PDE. We apply RONS to the Euler equation for ideal fluids, Navier-Stokes equations for incompressible flow, and shallow water equation modeling tsunamis. In each case, we discuss the effect of conserved quantities on the extreme events and energy fluxes and compare the results to conventional Galerkin truncations.

## [00308] Verifying global stability of fluid flows despite transient growth of energy

**Format :** Online Talk on Zoom

**Author(s) :** David Goluskin (University of Victoria)Federico Fuentes (Pontificia Universidad Católica de Chile)Sergei Chernyshenko (Imperial College London)

**Abstract :** To verify nonlinear stability of a laminar fluid flow against all perturbations, all past results rely on monotonic decrease of perturbation energy or a similar quadratic generalized energy. This "energy method" cannot show stability if perturbation energy can grow transiently, as in parallel shear flows at moderate Reynolds numbers. I will describe a more general approach that uses sum-of-squares polynomials to computationally construct non-quadratic Lyapunov functions that verify stability. Computational implementation for the example of 2D plane Couette flow verifies global stability at Reynolds numbers above the energy stability threshold found by Orr in 1907.

## [01836] Invariant solutions representing extreme behaviour in turbulence

**Format :** Talk at Waseda University

**Author(s) :** Genta Kawahara (Osaka University)

**Abstract :** Invariant solutions to the incompressible Navier-Stokes equations are reviewed to theoretically interpret extreme behaviour observed in turbulent flows. Turbulent bursting in near-wall turbulence is characterised in terms of homoclinic orbits to the periodic edge state at low Reynolds numbers, while it is discussed using another vigorous turbulent saddle at high Reynolds numbers. The ultimate state, i.e. anomaly of energy and scalar dissipation, of turbulent thermal convection is represented by steady solutions.

## [03543] Numerical simulation of the convex integration for the dissipative Euler flow

**Format :** Talk at Waseda University

**Author(s) :** Takeshi Matsumoto (Department of physics, Kyoto university)

**Abstract :** Weak solutions to the three-dimensional, incompressible Euler equations, which can dissipate the energy, were constructed with the convex integration by De Lellis, Szekelyhidi and collaborators. We develop a numerical simulation of the physically appealing construction by Buckmaster et al. Specifically, we study the solutions with the standard tools in physics of analyzing turbulent flows, such as the structure functions. We discuss insights obtained from them and also limitations of the simulation.

00263 (2/3) : 1D @D401 [Chair: Takeshi Matsumoto]

## [00597] Systematic search for singularities in 3D Euler flows

**Format :** Talk at Waseda University

**Author(s) :** Bartosz Protas (McMaster University)Xinyu Zhao (McMaster University)

**Abstract :** We consider the question about formation of singularities in incompressible Euler flows. Based on the local well-posedness result guaranteeing existence of smooth solutions in the Sobolev space  $H^m$ ,  $m > 5/2$ , we search for potentially singular flows systematically by solving a PDE optimization problem where the  $H^3$  norm is maximized at time  $T$ . Solutions of this problem obtained using an adjoint-based gradient descent method indicate the possibility of singularity formation if the time  $T$  is sufficiently long.

## [00371] Mathematical reformulation of the Kolmogorov-Richardson energy cascade in terms of vortex stretching and related topics

**Format :** Talk at Waseda University

**Author(s) :** Tsuyoshi Yoneda (Hitotsubashi University)Susumu Goto (Osaka University)Tomonori Tsuruhashi (University of Tokyo)

**Abstract :** With the aid of direct numerical simulations of forced turbulence in a periodic domain, we mathematically reformulate the Kolmogorov-Richardson energy cascade in terms of vortex stretching. More precisely, under the assumptions of the scale-locally of the vortex stretching/compressing process and the statistical independence between vortices that are not directly stretched or compressed, we can derive the -5/3 power law of the energy spectrum of statistically stationary turbulence without directly using the Kolmogorov hypotheses.

## [03746] Structure and scaling of extremely large velocity gradients in hydrodynamic turbulence.

**Format :** Talk at Waseda University

**Author(s) :** Alain Pumir (CNRS and Ecole Normale Supérieure de Lyon) Dhawal Buaria (New York University)

**Abstract :** I will discuss extreme events in the velocity gradient tensor of turbulent flows, using data from Direct Numerical Simulations (DNS) of turbulent flows up to a Taylor-scale Reynolds number of 1300. I will review some essential properties of the velocity gradient tensor, and in particular, the dependence of the strain, conditioned on vorticity, and the dependence on the Reynolds number of the probability density functions of the vorticity and strain. These properties lead to the proposition of a simple framework to quantify the extreme events and the smallest scales of turbulence. This work accentuates the importance of the relation between strain and vorticity in developing an accurate understanding of intermittency in turbulence.

In exploring further this relation, I will discuss the unexpected role of strain for very intense vortices, and discuss the self-attenuation of intense vortices in DNS of turbulent flows.

## [00303] A model of turbulent flows based on a random Constantin-Lax-Majda-DeGregorio equation

**Format :** Talk at Waseda University

**Author(s) :** Takashi Sakajo (Kyoto University) Yuta Tsuji (Kyoto University)

**Abstract :** The generalized Constantin-Lax-Majda-DeGregorio (gCLMG) equation with the viscous dissipation under a large-scale forcing is utilized as a one-dimensional model of turbulent flows generating the cascade of the conserved quantity. In this talk, we show the global existence of a unique solution of the gCLMG equation subject to random forcing functions that are chosen from a given distribution. Moreover, we numerically investigate the solutions' statistical properties by Galerkin approximation of random variables with generalized Polynomial Chaos.

00263 (3/3) : 1E @D401 [Chair: Takashi Sakajo]

## [00786] Extending the Gibbon-Fokas-Doering stagnation-point-type ansatz to finite-energy initial conditions: A solution to the Navier-Stokes Millennium Prize Problem?

**Format :** Talk at Waseda University

**Author(s) :** Miguel David Bustamante (University College Dublin)

**Abstract :** The stagnation-point-type solution to the 3D incompressible Navier-Stokes equations found in {Gibbon, Fokas and Doering, (Physica A, D) **132**, 497 {1999}} produced an infinite family of solutions to the 3D incompressible Euler equations that blow up in a finite time. There is an exact formula for the singularity time as a functional of the initial conditions {Constantin, (Int. J., Math., Res., Not.) **2000**, 455 {2000}; Mulungye, Lucas and Bustamante, (J., Fluid, Mech.) **771**, 468 {2015}; \_\_\_, (J., Fluid, Mech.) **788**, R3 {2016}}, and the solutions to this and related models are best understood in terms of infinitesimal Lie symmetries {Bustamante, (Phil. Trans. R., Soc., A) **380**, 20210050 {2022}}. The main drawback of these solutions, *from the viewpoint of the Clay Millennium Prize*, is that the velocity field depends linearly on the out-of-plane spatial coordinate, and thus the initial condition has infinite energy. In this talk, I will present a way to extend these solutions in order to have an arbitrary dependence on the out-of-plane coordinate, allowing in principle for finite-energy solutions. This extension seems to break the infinitesimal Lie symmetry structure inherent to the previous infinite-energy solutions, so a statement regarding finite-time blowup is not yet available analytically in the finite-energy case. However, the extension allows for a novel numerical attempt at the finite-energy solution, via a hierarchy of systems of coupled 2D partial differential equations, which are much easier to handle than a full 3D problem. I will present results and prospects, and discuss potential applications to real-life experiments.

## [04968] Singularity detection via regularization: Blow-up criteria for 3D Euler and related equations

**Format :** Talk at Waseda University

**Author(s) :** Adam Larios (University of Nebraska-Lincoln) Edriss Titi (Texas A&M University) Isabel Safarik (University of Nebraska-Lincoln)

**Abstract :** The 3D Euler-Voigt equations can be thought of as a regularization of the 3D Euler equations in the sense that they are globally well-posed, and the solutions approximate the solutions to the 3D Euler equations. We describe a blow-up criterion for the 3D incompressible Euler equations based on inviscid Voigt regularization. Therefore, the blow-up criterion allows one to gain information about possible singularity formation in the 3D Euler equations indirectly; namely, by simulating the “better-behaved” 3D Euler-Voigt equations. Analytical and computational results will be discussed. We will also discuss applications to Navier-Stokes and a recent Voigt-type regularization and blow-up criterion based on the Velocity-Vorticity formulation of the 3D Navier-Stokes equations.

## [02897] Thermalisation in finite-dimensional, inviscid equations of hydrodynamics

**Format :** Talk at Waseda University

**Author(s) :** Samridhhi Sankar Ray (International Centre for Theoretical Sciences, Tata Institute of Fundamental Research (ICTS-TIFR)) Sugan D. Murugan (International Centre for Theoretical Sciences, Tata Institute of Fundamental Research (ICTS-TIFR))

**Abstract :** The question of thermalisation of classical systems with many degrees of freedom is a fundamentally important one in statistical physics. There are several examples of such systems, with explicitly broken integrability, which thermalise. A slightly different class of such systems which are even less understood are the finite-dimensional (Galerkin-truncated) equations of ideal hydrodynamics. The long time solutions of these equations thermalise---characterised by a Gibbs distribution of the velocity field and kinetic energy equipartition amongst its (finite) Fourier modes---by virtue of a phase-space and energy conservation and a simple application of Liouville's theorem. While this property has been long known, the precise mechanisms which trigger such states have only been discovered recently. In this talk we discuss this mechanism and show how there could be ways to prevent the onset of thermalisation and provide a way to tackle the important questions of finite-time blow-up and weak solutions numerically.

## [00758] How advection delays singularity formation in the Navier-Stokes equations

**Format :** Online Talk on Zoom

**Author(s) :** Koji Ohkitani (RIMS, Kyoto University)

**Abstract :** We numerically study the Navier-Stokes equations modified by depleting advection. In the inviscid case some solutions blow up in finite time when advection is discarded, Constantin 1986. We use a pair of orthogonally offset vortex tubes as initial data. We show that: 1) blowup persists even with viscosity when advection is discarded, and 2) the time of breakdown increases logarithmically as we reinstate advection, consistent with the regularity of the Navier-Stokes equations.

## [00264] Card-based Protocols and PEZ Protocols

**Session Time & Room :** 5D (Aug.25, 15:30-17:10) @A206

**Type :** Proposal of Minisymposium

**Abstract :** Secure computation protocols enable distrustful parties, each holding secret input, to compute a function of their inputs without revealing their inputs beyond the function value. Zero-knowledge protocols allow a prover to convince a verifier that there exists a solution to the puzzle without revealing the solution itself. While these cryptographic protocols are usually implemented on electronic computers, there is another line of research on cryptography using everyday physical objects instead of electronic devices. This mini-symposium will be devoted to so-called card-based protocols and PEZ protocols, which establish cryptographic tasks using a deck of physical cards and a PEZ dispenser, respectively.

**Organizer(s) :** Kazumasa Shinagawa, Kengo Miyamoto, Takaaki Mizuki

**Classification :** 94A60

**Minisymposium Program :**

00264 (1/1) : 5D @A206

## [04248] Physical ZKPs for Logic Puzzles Using a Standard Deck of Cards

**Author(s) :** Suthee Ruangwises (The University of Electro-Communications)

**Abstract :** Recently, many researchers have been focusing on constructing physical zero-knowledge proof (ZKP) protocols for logic puzzles using a deck of cards. However, all of the developed protocols so far require several identical copies of some cards, making them impractical. In this talk, we introduce more practical ZKP protocols for two of the most famous logic puzzles: Sudoku and Makaro, that can be implemented using a standard deck (a deck consisting of all different cards).

## [05000] Open Problems in Card-Based Cryptography

**Author(s)** : Alexander Koch (CNRS, IRIF)

**Abstract** : Card-based cryptographic protocols for secure multiparty computation allow to jointly compute a function, without giving anything away about someone's input that is not obvious from the output, using only a deck of cards. Since the five-card AND protocol of den Boer (EUROCRYPT 1989), this topic has developed into a full-blown research area. The talk identifies some open problems in card-based cryptography, with a focus on lower bounds on protocol parameters for different functions and models.

## [05052] Recent Progress in Card-Based Cryptography

**Author(s)** : Daiki Miyahara (The University of Electro-Communications / AIST)

**Abstract** : Research on card-based cryptography began with the five-card trick, invented in 1989, which computes the two-input logical AND function using a deck of five cards without revealing any information other than necessary. In this talk, I will first introduce it and provide an overview of the major trends in this line of research. Subsequently, I present recent work published in 2021 that deals with the three-input majority function employing the five-card trick.

## [05471] Introduction to Private PEZ Protocol

**Author(s)** : Yoshiki Abe (The University of Electro-Communications)

**Abstract** : A PEZ dispenser is a stack-like physical device. We explain the model and construction of the multiparty computation using a PEZ dispenser called private PEZ protocols. First, we will discuss the security requirements for private PEZ protocols by comparing secure and insecure protocols for computing the logical AND function. Then, we show the recursive structure in private PEZ protocols through an example of a three-input majority voting protocol.

# [00268] Neumann—Poincaré Operator, Layer Potential Theory, Plasmonics and Related Topics

**Session Time & Room :**

00268 (1/4) : 1E (Aug.21, 17:40-19:20) @G701

00268 (2/4) : 2C (Aug.22, 13:20-15:00) @G701

00268 (3/4) : 2D (Aug.22, 15:30-17:10) @G701

00268 (4/4) : 2E (Aug.22, 17:40-19:20) @G701

**Type** : Proposal of Minisymposium

**Abstract** : The Neumann—Poincaré operator (abbreviated by NP) is a boundary integral linear operator known as one of the important tools associated with boundary value problems in the field of partial differential equations. The detailed properties of NP operators can be comprehended as governing dynamics of many physical systems. Especially, the NP spectrum controls some physical systems (Electro dynamics, elastic systems and etc.) .

Our purpose here is to discuss the spectral structure of NP operators and their applications to physical systems.

N.B. We would like to hold 4 sessions at this minisymposium.

**Organizer(s)** : Kazunori Ando, Yoshihisa Miyanishi

**Classification** : 35P05, 31-06, Neumann--Poincaré operator, Spectrum

**Minisymposium Program :**

00268 (1/4) : 1E @G701 [Chair: Yoshihisa Miyanishi]

## [03110] Homogenization and the spectrum of the Neumann Poincaré operator

**Format** : Talk at Waseda University

**Author(s)** : Eric Bonnetier (Institut Fourier, Université Grenoble Alpes)

**Abstract** : Resonances of metallic nano-particles has been an active topic of investigation in the last decade, as this phenomenon allows localization of strong electro-magnetic fields in very small regions of space, an interesting feature for many applications. Asymptotically as the size of the particles tends to 0, the resonant frequencies are related to the spectral properties of the Neumann-Poincaré operator (NP).

In this talk, we discuss the spectrum of that integral operator, when one considers a periodic distribution of inclusions made of metamaterials in a dielectric background medium. The underlying question, is what can happen when many resonant particles interact ?

We show that under the assumptions that the inclusions are fully embedded in the periodicity cells, the spectra  $\sigma_\varepsilon$  of the NP operators for a collection of period  $\varepsilon$  converge to a limiting set composed of 2 parts : the union of the Bloch spectra of NP operators defined over periodicity cells with quasi-periodic boundary conditions and a boundary spectrum associated with eigenfunctions which spend a not too small part of their energy near the boundary.

This is joint work with Charles Dapogny and Faouzi Triki.

## [00406] From condensed matter theory to sub-wavelength physics

**Format :** Talk at Waseda University

**Author(s) :** Habib Ammari (ETH Zurich)

**Abstract :** The ability to manipulate and control waves at scales much smaller than their wavelengths is revolutionizing nanotechnology. The speaker will present a mathematical framework for this emerging field of physics and elucidate its duality with condensed matter theory.

## [00777] Eigenvalues of zero order pseudodifferential operators and applications to Neumann-Poincare

**Format :** Online Talk on Zoom

**Author(s) :** Grigori Rozenblioum (Chalmers University of Technology)

**Abstract :** The NP operator for 3D elasticity is a zero order pseudodifferential operator, polynomially compact for a homogeneous material. For such operators we study behavior of eigenvalues converging to the points of essential spectrum and find their relation with the geometry of the body. For a nonhomogeneous material the essential spectrum fills intervals, we study eigenvalues converging to the tips of the essential spectrum.

00268 (2/4) : 2C @G701 [Chair: Kazunori Ando]

## [00564] On a uniqueness property of harmonic functions

**Format :** Online Talk on Zoom

**Author(s) :** Dmitry Khavinson (University of South Florida)

**Abstract :** This is not a new result, yet the paper was dedicated to Walter Hayman and the main question , raised there is still unanswered. The paper was the joint work with late Harold S. Shapiro. We shall discuss the problem of uniqueness for functions  $u$  harmonic in a domain  $G$  in  $R^n$  and vanishing on some parts of the intersection  $V$  {not necessarily connected} of  $G$  with a line  $m$ . The question originated more than two decades ago with N. Nadirashvili {private communication}. For example, let  $G$  be a spherical shell, i.e., the region between two concentric spheres, and  $m$  is a line through the origin. Does  $u$  vanish on both segments along which  $m$  intersects  $G$  if it does so on one of them? To illustrate the cunning depth of the question note that if you let  $G$  to be the annulus with a sector cut out, the function  $u = \arg z$  in the plane does vanish on the positive part of the real axis, but not on the whole intersection. What happens if  $G$  is a spherical shell but  $m$  does NOT pass through the center? What if we replace harmonic functions by polyharmonic functions, or, more generally, solutions of analytic elliptic equations, or even worse, by linear combinations of Riesz potentials that satisfy no PDE altogether? The answers are by no means obvious and, in many cases, may be judged as surprising.

## [00367] Factorization of Neumann-Poincare operator

**Format :** Talk at Waseda University

**Author(s) :** Mihai Putinar (University of California)

**Abstract :** It is well known that the Neumann-Poincare operator (double layer potential) is symmetrizable. We will discuss a factorization of this singular integral operator which explains this essential spectral feature.

## [00452] The quasi-static plasmonic problem for polyhedra

**Format :** Talk at Waseda University

**Author(s) :** Karl-Mikael Perfekt (NTNU)

**Abstract :** I will present a characterization of the essential spectrum of the plasmonic problem for polyhedra in  $R^3$ . The description is particularly simple for convex polyhedra and relative permittivities  $\varepsilon < -1$ . The results are obtained through detailed analysis of the double layer potential for polyhedral cones and polyhedra.

Based on joint work with Marta de León-Contreras.

00268 (3/4) : 2D @G701 [Chair: Yoshihisa Miyanishi]

## [00364] Surface localized resonances and applications

**Format** : Talk at Waseda University

**Author(s)** : Hongyu Liu (City University of Hong Kong)

**Abstract** : In this talk, I shall discuss our recent discoveries on certain novel surface localized resonances which were inspired by the surface plasmon resonance. These localized resonances generate a variety of interesting applications.

## [01244] Spectral structure of the Neumann-Operator on thin domains

**Format** : Talk at Waseda University

**Author(s)** : Hyeonbae Kang (Inha University)

**Abstract** : The Neumann-Poincaré operator on thin domains, such as thin rectangles, thin prolate spheroids, flat oblate ellipsoids, exhibits interesting spectral structure. In this talk we review recent development on this topic.

## [00730] A unified approach to the field concentration problem

**Format** : Talk at Waseda University

**Author(s)** : Sanghyeon Yu (Korea University)

**Abstract** : Composite materials shows the high field concentration when the inclusions have geometric singularities in their boundaries. This phenomenon has many practical applications in imaging, spectroscopy, and meta-materials. In this talk, we discuss a new way of tackling the field concentration problem via the spectral analysis of the Neumann-Poincaré operator. We focus on two kinds of important singularities: nearly touching surfaces and high curvature points.

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00268 (4/4) : 2E @G701 [Chair: Yoshihisa Miyanishi]

## [00354] Spectral properties of the Neumann–Poincaré operator on rotationally symmetric domains

**Format** : Talk at Waseda University

**Author(s)** : Yong-Gwan Ji (Korea Institute for Advanced Study)Hyeonbae Kang (Inha University)

**Abstract** : In this talk, we will discuss the spectral properties of the Neumann-Poincaré operator when domains have rotational symmetry. We prove that if a domain  $\Omega$ , in two dimensions, has rotational symmetry then NP spectrum on  $\Omega$  contains NP spectrum on  $D$  which generates rotationally symmetric domain  $\Omega$  by  $m$ -th root transformation.

## [01245] Vector field decomposition and eigenvalues of elastic Neumann-Poincaré operators

**Format** : Talk at Waseda University

**Author(s)** : Shota Fukushima (Inha University)Yong-Gwan Ji (Korea Institute for Advanced Study)Hyeonbae Kang (Inha University)

**Abstract** : We show that all vector fields restricted to a surface is decomposed into three components and each component is characterized by the divergence-free or rotation-free harmonic extension to inside or outside of the domain. These three components correspond to three accumulation points of the eigenvalues of the elastic Neumann-Poincaré operator, which is a singular integral operator on the boundary.

## [01265] Essential spectrum of elastic Neumann-Poincaré operators with a corner

**Format** : Talk at Waseda University

**Author(s)** : Daisuke Kawagoe (Kyoto University)

**Abstract** : The elastic Neumann–Poincaré operator is a boundary integral operator naturally appearing when we solve the Lamé system in a bounded domain. For the two-dimensional case, if the boundary is smooth, then its spectrum consists of two sequences of eigenvalues with two accumulation points. In this talk, we consider the situation where the planar domain is smooth except at a corner and show that the essential spectrum appears around the above accumulation points.

**[00662] Fundamental solutions in Colombeau algebra****Format :** Talk at Waseda University**Author(s) :** Nobuto Yoneyama (Shinshu university)Yoshihisa Miyanishi (Shinshu University)**Abstract :** The notion of fundamental solutions {abbreviated by FS} is introduced in Colombeau algebra. Then we can construct a little more generalized FS even for Lewy-type equation whereas there are no FS in the sense of distributions.**[00276] Interplay of Numerical and Analytical Methods in Nonlinear PDEs****Session Time & Room :**

00276 (1/2) : 1C (Aug.21, 13:20-15:00) @G502

00276 (2/2) : 1D (Aug.21, 15:30-17:10) @G502

**Type :** Proposal of Minisymposium**Abstract :** Devising reliable numerical schemes and analytically understanding fine properties of solutions of nonlinear partial differential equations are challenging mathematical tasks. Theoretically and practically relevant examples are geometrically constrained PDEs such as harmonic maps and isometric bending problems. Modern applications arise in the development of new storage technologies and micro tools. Numerical simulations provide valuable experimental insight that can motivate analytical results, e.g. about singularities. Conversely, stability results for solutions lead to convergence theories for numerical schemes. The minisymposium aims at bringing together scientists from analysis and numerics working on nonlinear PDEs in order to inspire new mathematical developments.**Organizer(s) :** Sören Bartels, Diane Guignard, Christof Melcher**Classification :** 35Bxx, 65Nxx, 49Jxx**Minisymposium Program :**

00276 (1/2) : 1C @G502 [Chair: Christof Melcher]

**[05323] Hartree-Fock theory with a self-generated magnetic field****Format :** Talk at Waseda University**Author(s) :** Carlos J. Garcia Cervera (UCSB)Rafael Lainez Reyes (UCSB)**Abstract :** The study of a quantum system of N electrons interacting with K nuclei through the Coulomb potential has a long history in the mathematics community. In the first part of my talk, I will go over some of the quantum mechanical models developed to describe these systems, focusing on their mathematical structure and properties.

Following that, I will describe how these theories change when a magnetic field is present. In particular, I will define the Hartree-Fock ground state problem for a system of N electrons and K nuclei in the presence of self-generated magnetic fields and direct coupling and we will study the existence of the ground state and excited states, as well as some numerical approaches for its computation. The work I present is in collaboration with Rafael Lainez Reyes.

**[02913] Uniform flow in axisymmetric devices through permeability optimization****Format :** Online Talk on Zoom**Author(s) :** Harbir Antil (George Mason University)Drew P Kouri (Sandia National Labs)Denis Ridzal (Sandia National Labs)David Robinson (Sandia National Labs)Maher Salloum (Sandia National Labs)**Abstract :** Porous media enable the intimate contact between a fluid and a functional solid that can accomplish tasks valuable to chemical engineers, such as catalytic reaction, chemical separations, chemical species detection, and filtration. New additive manufacturing technologies enable the creation of porous media with precise control of the geometry of each pore, which could enable improved performance and more flexible design of chemical engineering devices. However, new design tools are needed to accomplish this. In this talk, we analyze an optimization problem, constrained by Darcy's law, to design porous media columns that achieve uniform fluid flow properties despite having nonuniform geometries. We prove existence of solutions to our problem, as well as differentiability, which enables the use of rapidly converging, derivative-based optimization methods. We demonstrate our approach on two

axisymmetric columns where we achieve a desired velocity field with uniform transit times despite varying device cross sections.

## [03496] Regularised stochastic Landau-Lifshitz equations and their application in numerical analysis

**Format :** Talk at Waseda University

**Author(s) :** Chunxi Jiao (RWTH Aachen University )

**Abstract :** We revisit a regularised stochastic Landau-Lifshitz equation (sLLE) with bi-Laplacian in the effective field and study a similarly regularised stochastic Landau-Lifshitz-Bloch equation (sLLBE) in a two-dimensional domain. We derive the rate of convergence (in probability) of numerical solutions of a finite-element scheme for the regularised sLLBE to the solution of sLLBE, and outline the difficulty of applying this approach to sLLE. This talk is based on a joint work with Benjamin Goldys and Ngan Le.

## [03482] A least squares Hessian/Gradient recovery method for fully nonlinear PDEs in Hamilton--Jacobi--Bellman form

**Format :** Talk at Waseda University

**Author(s) :** Omar Lakkis (University of Sussex)Amireh Mousavi (Jena Universität)

**Abstract :** Least squares recovery methods provide a simple and practical way to approximate linear elliptic PDEs in nondivergence form where standard variational approach either fails or requires technically complex modifications. This idea allows the creation of relatively efficient solvers for fully nonlinear elliptic equations, the linearization of which leaves us with an equation in nondivergence form. An important class of fully nonlinear elliptic PDEs is that of Hamilton--Jacobi--Bellman form.

Suitable functional spaces and penalties in the cost functional must be carefully crafted in order to ensure stability and convergence of the scheme with a good approximation of the gradient and Hessian which is useful, for example, for Newton--Raphson, semismooth Newton, or a policy iteration (Howard) approximation of a Hamilton--Jacobi--Bellman equation. We prove convergence and provide convergence rates under a Cordes condition.

00276 (2/2) : 1D @G502 [Chair: Diane Guignard]

## [01636] Convergent finite element approximation of liquid crystal polymer networks

**Format :** Talk at Waseda University

**Author(s) :** Shuo Yang (Yanqi Lake Beijing Institute of Mathematical Sciences and Applications)Ricardo Nochetto (University of Maryland)Lucas Bouck (University of Maryland)

**Abstract :** Liquid crystals polymer networks (LCN) deform spontaneously upon temperature or optical actuation. In this talk, we discuss a 2D membrane model of LCN and its properties. We design a finite element discretization for this model, propose a novel iterative scheme to solve the non-convex discrete minimization problem, and prove stability of the scheme and a convergence of discrete minimizers. We present a wide range of numerical simulations.

## [01583] Evolving FEMs with artificial tangential velocities for curvature flows

**Format :** Talk at Waseda University

**Author(s) :** Jiashun Hu (Hongkong Polytechnic University)Buyang Li (Hongkong Polytechnic University)

**Abstract :** By considering a limiting situation in the method proposed by Barrett, Garcke and Nurnberg, a new artificial tangential velocity is introduced into the evolving finite element methods for mean curvature flow and Willmore flow to improve the mesh quality of the numerically computed surfaces. Stability and optimal-order convergence of the evolving finite element methods are established.

## [03481] Finite element approximation of implicitly constituted non-Newtonian fluids

**Format :** Online Talk on Zoom

**Author(s) :** Endre Suli (University of Oxford)

**Abstract :** The framework of classical continuum mechanics, built upon an explicit constitutive equation for the stress tensor, is too narrow to describe inelastic behaviour of solid-like materials or viscoelastic properties of materials. We

present a survey of recent results concerning the mathematical analysis of finite element approximations of implicit power-law-like models for viscous incompressible fluids, where the stress tensor and the symmetric part of the velocity gradient are related by a, possibly multi-valued, maximal monotone graph.

## [01330] Error analysis for a local discontinuous Galerkin approximation for systems of p-Navier–Stokes type

**Format :** Talk at Waseda University

**Author(s) :** Alex Kaltenbach (University of Freiburg)

**Abstract :** In this talk, we propose a Local Discontinuous Galerkin (LDG) approximation for systems of p-Navier–Stokes type involving a new numerical flux in the stabilization term and a new discretization of the convective term. A priori error estimates are derived for the velocity, which are optimal for all  $p > 2$  and  $\delta \geq 0$ . A new criterion is presented that yields a priori error estimates for the pressure, which are optimal for all  $p > 2$  and  $\delta \geq 0$ .

## [00278] Nonlocal Modeling, Analysis, and Computation

**Session Time & Room :**

00278 (1/4) : 2C (Aug.22, 13:20-15:00) @G406

00278 (2/4) : 2D (Aug.22, 15:30-17:10) @G406

00278 (3/4) : 2E (Aug.22, 17:40-19:20) @G406

00278 (4/4) : 3C (Aug.23, 13:20-15:00) @G406

**Type :** Proposal of Minisymposium

**Abstract :** The past decade has seen a rapid growth in the development of nonlocal mathematical models. Nonlocal modeling is now being used in applications including continuum mechanics and fracture mechanics, anomalous diffusion and advection diffusion, and other fields. This minisymposium seeks to bring together mathematicians and domain scientists from different disciplines working on nonlocal modeling and is intended to serve as an international forum for the state of the art in the modeling, analysis, and numerical aspects of nonlocal models.

**Organizer(s) :** Patrick Diehl, Pablo Seleson, Robert Lipton, Qiang Du

**Classification :** 35axx, 49-xx, 65-xx

**Minisymposium Program :**

00278 (1/4) : 2C @G406 [Chair: Patrick Diehl]

## [02501] Coarse-Graining and Nonlocality

**Format :** Online Talk on Zoom

**Author(s) :** Stewart A Silling (Sandia National Laboratories)

**Abstract :** The most intuitive applications of nonlocal modeling arise when long-range interactions, such as electrostatic fields, are present in a physical system. However, nonlocal descriptions are also produced by the homogenization or coarse-graining of heterogeneous, small-scale systems. In this talk, it is shown that the coarse-graining of molecular systems or of local, elastic, heterogeneous systems leads to the peridynamic nonlocal linear momentum balance. Examples demonstrate the discovery of nonlocal material models applicable to a coarse-grained description.

## [00366] Wellposedness, regularity, and convergence of nonlocal solutions to classical counterparts

**Format :** Talk at Waseda University

**Author(s) :** Petronela Radu (University of Nebraska-Lincoln)

**Abstract :** The successful employment of nonlocal models in a variety of applications relies on a deep understanding of mathematical properties and analysis of the underlying integral operators and associated systems of equations. In this talk I will present some recent results on nonlocal frameworks systems based on some existing, as well as newly introduced, nonlocal operators. The studies include a series of results on nonlocal versions of integration by parts

theorems, boundary conditions (both, Dirichlet and Neumann), Helmholtz-Hodge type decompositions, as well as convergence of operators to their classical equivalents as the interaction horizon vanishes.

## [00370] Coupling of an atomistic model and peridynamic model using an extended Arlequin framework

**Author(s)** : Jieqiong Zhang (Northwest University )Fei Han (Dalian University of Technology)

**Abstract** : A general nonlocal coupling technique between an atomistic (AM) model and the bond-based peridynamic (PD) model is proposed, based on the Arlequin framework. This technique applies the complementary weight function and constraint conditions to transmit energies through the overlapping region between the AM and PD regions. We extend the original Arlequin framework to discrete cases by redefining constraint conditions by the peridynamic differential operator, which enables the interpolation and corresponding derivative of scattered data. Besides, the preconditioning of calibration for the PD effective micromodulus is implemented to guarantee the equilibrium of energy. One-dimensional benchmark tests investigate the coupling effects influenced by several key factors, including the coupling length, weight function, grid size and horizon in the PD model, and constraint conditions. Two- and three-dimensional numerical examples are provided to verify the applicability and effectiveness of this coupling model. Results illustrate this AM-PD coupling model takes the mutual advantages of the computational efficiency of PD model and the accuracy of AM model, which provides a flexible extension of the Arlequin framework to couple particle methods.

## [00445] Local and nonlocal energy-based coupling models

**Format** : Talk at Waseda University

**Author(s)** : Julio D. Rossi (Buenos Aires Univ.)

**Abstract** : In this talk we will present two different ways of coupling a local operator with a nonlocal one in such a way that the resulting equation is related to an energy functional.

In the first strategy the coupling is given via source terms in the equation and in the second one a flux condition in the local part appears.

For both models we prove existence and uniqueness of a solution that is obtained via direct minimization of the related energy functional.

In the second part of this talk we extend these ideas to deal with local/nonlocal elasticity models in which we couple classical local elasticity with nonlocal peridynamics.

joint work with G. Acosta and F. Bersetche.

00278 (2/4) : 2D @G406 [Chair: Patrick Diehl]

## [01086] Machine-learning based coupling of local and nonlocal models

**Format** : Talk at Waseda University

**Author(s)** : Patrick Diehl (LSU)Noujoude Nader (LSU)Serge Prudhomme (PolyMTL)

**Abstract** : This talk will present a machine-learning coupling approach for local and nonlocal models. We will identify when to switch two the coupled system and where to place the nonlocal region within the local region. We will present some one-dimensional and two-dimensional examples to showcase the applicability of the approach.

## [01235] Nonlocal Neural Operators for Learning Complex Physical Systems with Momentum Conservation

**Format** : Online Talk on Zoom

**Author(s)** : Yue Yu (Lehigh University)

**Abstract** : Neural operators have recently become popular tools for learning responses of complex physical systems. Nevertheless, their applications neglects the intrinsic preservation of fundamental physical laws. Herein, we introduce a novel integral neural operator architecture, to learn physical models with conservation laws of linear and angular momentums automatically guaranteed. As applications, we demonstrate our model in learning complex material behaviors from both synthetic and experimental datasets, and show that our models achieves state-of-the-art accuracy and efficiency.

## [03023] A Numerical Study of the Peridynamic Differential Operator Discretization of Incompressible Navier-Stokes Problems

**Format :** Online Talk on Zoom

**Author(s) :** Burak Aksoylu (Texas A&M University-San Antonio)Fatih Celiker (Wayne State University)

**Abstract :** We study the incompressible Navier-Stokes equations using the Projection Method. The applications of interest are the classical channel flow problems such as Couette, shear, and Poiseuille. In addition, we consider the Taylor-Green vortex and lid-driven cavity applications. For discretization, we use the Peridynamic Differential Operator (PDDO). The main emphasis of the paper is the performance of the PDDO as a discretization method under these flow problems. We present a careful numerical study with quantifications and report convergence tables with convergence rates. We also study the approximation properties of the PDDO and prove that the  $N$ -th order PDDO approximates polynomials of degree at most  $N$  exactly. As a result, we prove that the PDDO discretization guarantees the zero row sum property of the arising system matrix.

## [03546] An efficient peridynamics-based coupling method for composite fracture

**Format :** Talk at Waseda University

**Author(s) :** Zihao Yang (Northwestern Polytechnical University)

**Abstract :** In this talk, we will introduce a peridynamics-based statistical multiscale framework and related numerical algorithms to predict the fracture of composite structure with randomly distributed particles. The heterogeneities of composites, including the shape, spatial distribution and volume fraction of particles, are characterized within the representative volume elements, and their impact on structure failure are extracted as two types of peridynamic parameters, namely, statistical critical stretch and equivalent micromodulus. Two- and three-dimensional numerical examples illustrate the validity, accuracy and efficiency of the proposed method.

00278 (3/4) : 2E @G406

## [03632] Nonlocal Boundary Value Problems with Local Boundary Conditions

**Author(s) :** James Scott (Columbia University)

**Abstract :** We state and analyze classical boundary value problems for nonlocal operators. The model takes its horizon parameter to be spatially dependent, vanishing near the boundary of the domain. We show the variational convergence of solutions to the nonlocal problem with mollified Poisson data to the solution of the localized classical Poisson problem with  $H^{-1}$  data as the horizon uniformly converges to zero. Several classes of boundary conditions are considered.

## [03718] On the optimal control of a linear peridynamic model

**Format :** Talk at Waseda University

**Author(s) :** Tadele Mengesha (University of Tennessee Knoxville )Abner Salgado (University of Tennessee Knoxville )Joshua Siktar (University of Tennessee Knoxville )

**Abstract :** We present a result on a non-local optimal control problem involving a linear, bond-based peridynamics model.

In addition to proving existence and uniqueness of solutions to our problem, we investigate their behavior as the horizon parameter, which controls the degree of nonlocality, approaches zero. We then study a finite element-based discretization of this problem, its convergence, and the so-called asymptotic compatibility as the discretization parameter and the horizon parameter vanish simultaneously.

## [03800] Nonlocal half-ball vector operators and their applications to nonlocal variational problems

**Author(s) :** Xiaochuan Tian (UC San Diego)Zhaolong Han (UC San Diego)

**Abstract :** Motivated by the growing interests in nonlocal models, and particularly peridynamics, we present a nonlocal vector calculus framework defined using the half-ball gradient, divergence, and curl operators. Theoretical developments of the nonlocal half-ball vector operators include nonlocal vector identities, nonlocal Poincaré inequality on bounded domains, and Bourgain-Brezis-Mironescu type compactness results. As a result, well-posedness of nonlocal variational problems can be obtained, and the applications include nonlocal convection-diffusion problems and the peridynamics correspondence model. In particular, we illustrate that the new peridynamics correspondence model defined by the half-ball vector operator is energy stable which removes the known zero-energy mode instability issue of peridynamics correspondence models.

## [05210] CabanaPD: A meshfree GPU-enabled peridynamics code for exascale fracture simulations

**Format :** Online Talk on Zoom

**Author(s) :** Pablo Seleson (Oak Ridge National Laboratory)Sam Reeve (Oak Ridge National Laboratory)

**Abstract :** Peridynamics is a nonlocal reformulation of classical continuum mechanics suitable for material failure and damage simulation, which has been successfully demonstrated as an effective tool for the simulation of complex fracture phenomena in many applications. However, the nonlocal nature of peridynamics makes it highly computationally expensive, compared to classical continuum mechanics, which often hinders large-scale fracture simulations. In this talk, we will present ongoing efforts to develop CabanaPD, a meshfree GPU-enabled peridynamics code for large-scale fracture simulations. CabanaPD is built on top of two main libraries: Kokkos and Cabana, both developed throughout the Exascale Computing Project (ECP). CabanaPD is performance-portable and exascale-capable, and it is designed to run on U.S. Department of Energy's supercomputers, including the newly deployed Frontier, which is the first exascale machine and today's top supercomputer worldwide.

00278 (4/4) : 3C @G406

## [00280] Canonical Scattering Theory and Application

**Session Time & Room :**

00280 (1/2) : 3D (Aug.23, 15:30-17:10) @D403

00280 (2/2) : 3E (Aug.23, 17:40-19:20) @D403

**Type :** Proposal of Minisymposium

**Abstract :** A resurging interest in metamaterials, in particular acoustic metamaterials, comprising multi-scale rigid, porous, and/or elastic materials with subwavelength resonators renews the need for a mathematical theory capable of dealing with wave interactions with such objects. This session will comprise advances across a range of canonical scattering and diffraction problems applicable to acoustic metamaterials. This lays the foundation for understanding and exploiting these materials across a range of industrial applications such as sound absorbent linings, acoustic cloaking devices, and acoustic lensing

**Organizer(s) :** Lorna Ayton

**Classification :** 76Qxx, 74Jxx, 78Axx, 35Jxx, 35Qxx

**Minisymposium Program :**

00280 (1/2) : 3D @D403 [Chair: Lorna Ayton]

## [02735] Diffraction of acoustic waves by multiple independent semi-infinite arrays.

**Format :** Talk at Waseda University

**Author(s) :** Matthew Allan Nethercote (University of Manchester)Raphael Assier (University of Manchester)Anastasia Kisil (University of Manchester)

**Abstract :** We consider multiple wave scattering problems with several semi-infinite periodic arrays of point scatterers. For each array, a coupled system of equations must be satisfied by the scattering coefficients. All of these systems are solved using the discrete Wiener-Hopf technique and the result leads to a invertible matrix equation. In particular, we look at two arrays forming a wedge interface and will make comparisons with numerical methods that do not rely on the array periodicity.

## [05383] Extending the Unified Transform Method for Periodic Scattering Problems

**Format :** Talk at Waseda University

**Author(s) :** Shiza Batool Naqvi (University of Cambridge)Lorna Ayton (University of Cambridge)

**Abstract :** The Unified Transform method (also known as Fokas method) is employed in unbounded convex domains to model wave scattering governed by the Helmholtz equation. The method is extended to consider periodic boundary conditions allowing for computation of infinite scattering patterns which have been previously studied using periodic

Green's functions and large-dimension Wiener--Hopf matrices. The method is amenable to impedance and elastic surfaces. Furthermore, complex arrangements of scatterers, such as non-parallel cascading plates, are considered.

## [01576] A Mathematical Method to Solve Diffraction Problems with Generalised Linear Boundary Conditions

**Format :** Talk at Waseda University

**Author(s) :** Alistair Hales (University of Cambridge)

**Abstract :** The Wiener—Hopf Technique is a popular method used in the analysis of diffraction problems and elsewhere. We present a novel methodology that can solve the gust diffraction problem for a surface with a general linear boundary condition, with the view of applying said solutions to leading or trailing edge noise problems for general (possibly non-rigid) materials.

We discuss how solving such a problem is primarily difficult due to the factorization procedure required for the Wiener—Hopf technique to work. However, such boundary conditions may be simplified using a transformation of variables to a trigonometric polynomial, whose roots give the information required to split the scalar kernel into individual factors. This methodology provides insight into the underlying structure of the kernel while also allowing numerical methods to be easily applied thanks to the Maliuzhinets function that originates from wedge diffraction problems.

As an initial demonstration of the theory, we compare different canonical choices for impedance boundaries and demonstrate not only how changing the impedance of the surface can affect the solution, but how choosing a correct boundary condition initially may prove cruci

## [03068] Acoustic emission of a vortex ring near a porous edge

**Format :** Talk at Waseda University

**Author(s) :** Huansheng Chen (Lehigh University)Zachary Yoas (General Dynamics Electric Boat)Mitchell Swann (Applied Research Laboratory, Pennsylvania State University)Justin Jaworski (Lehigh University)Michael Krane (Applied Research Laboratory, Pennsylvania State University)

**Abstract :** The sound of a vortex ring in a quiescent fluid passing near a semi-infinite porous edge is investigated analytically to determine its time-dependent pressure signal and directivity in the acoustic far field as a function of a single dimensionless parameter. Results for this configuration furnish an analogue to scaling results from standard trailing-edge noise analyses and permit a direct comparison to companion experiments that circumvent measurement contamination by background noise sources of a mean flow.

00280 (2/2) : 3E @D403 [Chair: Lorna Ayton]

## [03187] Spectral computations for defect scattering in disordered topological insulators

**Format :** Talk at Waseda University

**Author(s) :** Andrew Horning (Massachusetts Institute of Technology)Matthew Colbrook (University of Cambridge)Kyle Thicke (Texas A&M University)Alex Watson (University of Minnesota)

**Abstract :** Topological insulators (TIs) support remarkable electronic wave phenomena that persist even in the presence of material defects and disorder. However, these phenomena are governed by an infinite-dimensional Hamiltonian with exotic spectral properties, which has frustrated the development of rigorous computational methods for disordered TIs. We use recent advances in computational spectral theory to rigorously and efficiently calculate conductivities and the generalized eigenstates that mediate interfacial electronic transport in two-dimensional TIs.

## [02368] Analysis of oversampled collocation methods for wave scattering problems

**Format :** Talk at Waseda University

**Author(s) :** Georg Maierhofer (Sorbonne Université)

**Abstract :** In this talk, we will explore the extent to which the convergence properties of collocation methods for Fredholm integral equations can be improved by least-squares oversampling. We provide rigorous analysis to show that superlinear oversampling can enhance the convergence rates of the collocation method and reduce its sensitivity to the distribution of collocation points. We support our analysis with several numerical examples for the two-dimensional Helmholtz equation. This is joint work with Daan Huybrechs.

## [03067] Revisiting the frozen-gust assumption for edge scattering using spatially-varying wavepackets

**Format :** Talk at Waseda University

**Author(s) :** Sonya Tiomkin (Lehigh University) Justin Jaworski (Lehigh University)

**Abstract :** An analytic solution for the noise generated by a wavepacket traveling near the edge of a rigid semi-infinite flat plate is determined in closed form in the time domain. The spatially-varying wavepacket constitutes a surrogate model for turbulent flow distortions engendered by the edge geometry. This approach permits a relaxation of the common frozen gust assumption for trailing-edge noise prediction, whereby the local vorticity is assumed to be unaffected by the edge.

## [03239] Green's function for wave scattering by a semi-infinite flat plate with a serrated edge

**Format :** Talk at Waseda University

**Author(s) :** Benshuai Lyu (Peking University)

**Abstract :** An analytical Green's function is developed to study the wave scattering by a semi-infinite flat plate with a serrated edge. The scattered pressure is solved using the Wiener-Hopf technique in conjunction with the adjoint technique. The kernel decomposition can be performed analytically in the high-frequency regime, which yields closed-form analytical Green's functions for any arbitrary piecewise linear serrations. The Green's function is shown to agree well with Finite Element Method (FEM) computations at high frequencies.

# [00283] Recent developments in mathematical imaging and modeling in magnetic particle imaging

**Session Time & Room :**

00283 (1/3) : 4D (Aug.24, 15:30-17:10) @G301

00283 (2/3) : 4E (Aug.24, 17:40-19:20) @G301

00283 (3/3) : 5B (Aug.25, 10:40-12:20) @G301

**Type :** Proposal of Minisymposium

**Abstract :** Mathematical imaging and modeling are two key challenges in the imaging modality magnetic particle imaging (MPI). MPI provides reconstructions of the concentration of magnetic nanoparticles in 4D. To address this inverse problem properly, various dynamics need to be taken into account, e.g., the particles' magnetization behavior and the dynamics in the fluid tracer. MPI provides challenging problems in imaging, modeling, and parameter identification. In this mini-symposium, we aim at bringing together researchers working on MPI and related mathematical fields. We cover theoretical and practical topics focusing on mathematical and physical as well as algorithmic and computational issues.

**Organizer(s) :** Christina Brandt, Tobias Kluth

**Classification :** 00A69, 92C55, 78A46, Applied inverse problems

**Minisymposium Program :**

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00283 (1/3) : 4D @G301 [Chair: Christina Brandt]

## [03274] The image reconstruction problem in magnetic particle imaging and an application of the deep image prior

**Format :** Talk at Waseda University

**Author(s) :** Tobias Kluth (University of Bremen)

**Abstract :** Magnetic particle imaging (MPI) is a tracer-based imaging modality detecting the concentration of superparamagnetic iron oxide nanoparticles. The imaging problem is a linear inverse problem given by a Fredholm integral equation of the first kind describing the concentration-to-voltage mapping. The talk provides a general introduction to MPI and the imaging problem. We further investigate general deep image prior concepts for inverse problems and their application to image reconstruction in MPI.

## [05253] A hybrid model for image reconstruction in MPI using a FFL

**Format :** Online Talk on Zoom

**Author(s) :** Jürgen Frikel (OTH Regensburg)

**Abstract :** In Magnetic Particle Imaging (MPI), most model-based reconstruction methods rely on idealized assumptions, such as an ideal field-free line (FFL) topology. However, real MPI scanners generate magnetic fields with distortions that often lead to inaccurate reconstructions and artifacts. To improve the reconstruction quality in MPI, it is essential to develop more realistic models. In this talk, we present a hybrid MPI model that can integrate real measurements of the applied magnetic fields into a physical model. Based on this model, we introduce a novel calibration procedure that allows the acquisition of the required magnetic field measurements, independent of the resolution, and with significantly less time consumption than a measurement-based model. In addition, we present a discretization strategy for the model that can be used in algebraic reconstructions.

## [04125] MPI using an FFL-scanner: Radon-based image reconstruction for realistic setup assumptions

**Format :** Talk at Waseda University

**Author(s) :** Stephanie Blanke (Universität Hamburg)Christina Brandt (Universität Hamburg)

**Abstract :** Magnetic particle imaging is a tracer-based imaging modality exploiting the nonlinear magnetization response of magnetic particles to changing magnetic fields. We adapt forward model and reconstruction methods towards more realistic setup assumptions for the specific choice of using a field-free line scanner. In this case, the scanning geometry resembles those of computerized tomography and we are able to jointly reconstruct particle concentration and corresponding Radon data by means of total variation regularization.

## [04651] Parameter estimation for modeling of nanoparticle dynamics

**Format :** Online Talk on Zoom

**Author(s) :** Hannes Albers (Universität Bremen)Tobias Kluth (University of Bremen)

**Abstract :** In order to overcome the limitations of needing full delta probe calibrations for MPI, accurate and fast model-based image reconstruction with as few as possible calibration measurements are highly desirable. We discuss methods for estimating particle parameters from calibration measurements and subsequently applying them to dynamic particle models, such as the Néel relaxation model, to obtain modeled system matrices of high quality for reconstruction.

00283 (2/3) : 4E @G301 [Chair: Tobias Kluth]

## [05030] Implicit neural representations for super-resolution in magnetic particle imaging

**Format :** Talk at Waseda University

**Author(s) :** Franziska Schrank (RWTH Aachen University)Volkmar Schulz (RWTH Aachen University)

**Abstract :** Magnetic particle imaging is a medical imaging technology based on the non-linear magnetization of magnetic nanoparticles. For image reconstruction, the received signal from the excitation of the nanoparticles is converted into the particles' concentration distribution via the system matrix, which is commonly measured in a calibration scan. We propose to parametrize this system matrix using implicit neural representations, enabling to super-resolve it or to reduce the matrix' acquisition time by processing an undersampled matrix.

## [05026] Reducing displacement artifacts in multi-patch magnetic particle imaging

**Format :** Online Talk on Zoom

**Author(s) :** Marija Boberg (University Medical Center Hamburg-Eppendorf)Tobias Knopp (University Medical Center Hamburg-Eppendorf)Martin Möddel (University Medical Center Hamburg-Eppendorf)

**Abstract :** Magnetic particle imaging determines the spatial distribution of superparamagnetic nanoparticles within a small field-of-view. Multi-patch approaches can expand the field-of-view at the cost of artifacts caused by field imperfections. Time-consuming calibration scans can reduce these displacement artifacts by measuring system matrices for each patch. In this contribution, only one central system matrix is used, which is warped according to the underlying magnetic fields, resulting in low calibration times and higher image quality.

## [05158] Deconvolution of direct Chebyshev reconstructions in MPI with neural networks

**Format :** Online Talk on Zoom

**Author(s) :** Mathias Eulers (Universität zu Lübeck)Marco Maass (Universität zu Lübeck)Christine Drogik (Universität zu Lübeck)Alfred Mertins (Universität zu Lübeck)

**Abstract :** Recently, a direct reconstruction method using Chebyshev polynomials for multi-dimensional MPI has been proposed. The reconstruction method weights and sums the frequency components of the voltage signals with tensor products Chebyshev polynomials, followed by a deconvolution step to perform a very fast image reconstruction. Unfortunately, the method is degraded by image artifacts. In this presentation, the method itself will be explained and a data-driven deconvolution model is presented which improves the image quality.

00283 (3/3) : 5B @G301 [Chair: Tobias Kluth]

## [04792] A Flexible Approach to Model-Based Reconstruction in Magnetic Particle Imaging

**Format :** Talk at Waseda University

**Author(s) :** Thomas März (Hochschule Darmstadt)

**Abstract :** In Magnetic Particle Imaging (MPI) images are usually reconstructed using a system matrix obtained via a time-consuming calibration procedure.

Our approach employs a mathematical model based on the MPI signal encoding and its analytical properties.

We present our two-stage algorithm:

First stage: we estimate components of the MPI Core Operator by using a variational formulation.

Second stage: the image is reconstructed by regularized deconvolution while fitting the results of the first stage.

We demonstrate the performance of our algorithm with simulated data.

## [04806] Reconstruction of Dynamic Concentrations with Sequential Subspace Optimization

**Format :** Talk at Waseda University

**Author(s) :** Marius Nitzsche (University of Stuttgart)

**Abstract :** Magnetic particle imaging faces challenges in dealing with dynamics, which often results in motion artifacts and lower quality reconstructions due to limited averaging. Standard algorithms cannot produce high-quality images under these circumstances. To address these issues, we utilize the Regularized Sequential Subspace Optimization (Resesop) algorithm, which can account for model imperfections caused by motion without requiring strong prior information. We demonstrate the effectiveness of Resesop on both simulated and real dynamic MPI data.

## [04730] Joint motion estimation and image reconstruction for dynamic MPI

**Format :** Talk at Waseda University

**Author(s) :** Christina Brandt (Universität Hamburg)Lena Zdun (Universität Hamburg)

**Abstract :** Potential applications of MPI include highly dynamic tasks as blood flow imaging and instrument tracking during interventions. In this talk, we propose to tackle the additional challenges caused by the dynamics by a joint image reconstruction and motion estimation approach. We combine a multi-scale motion estimation algorithm with a stochastic primal-dual algorithm for image reconstruction. Convincing numerical results are achieved on in-vitro and in-vivo data using motion models matching the specific application.

## [00286] Low-Reynolds-number swimming: modelling, analysis and applications

**Session Time & Room :**

00286 (1/2) : 2D (Aug.22, 15:30-17:10) @A510

00286 (2/2) : 2E (Aug.22, 17:40-19:20) @A510

**Type :** Proposal of Minisymposium

**Abstract :** Swimming in a fluid at microscopic scale is at the heart of many questions pertaining to biology, soft matter physics and micro-robotics.

It usually involves a complex balance of hydrodynamics, elasticity and internal activity, yielding a wide range of issues requiring various mathematical viewpoints, from modelling the fluid-structure interaction to optimal propulsion and efficient control of the swimmer's trajectory, with perspectives on future applications to biomedical micro-robots. This minisymposium brings together a group of young and experienced researchers to share their contributions to some of the latest developments in the theoretical and numerical analysis of micro-swimmers.

**Organizer(s) :** Jessie Levillain, Clément Moreau

**Classification :** 76-10, 74F10, 92C70

**Minisymposium Program :**

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00286 (1/2) : 2D @A510 [Chair: Clément Moreau]

## [03028] Results on Classical Elastohydrodynamics for a Swimming Filament

**Format :** Talk at Waseda University

**Author(s) :** Laurel A Ohm (University of Wisconsin--Madison)

**Abstract :** We consider two models of an immersed inextensible filament undergoing planar motion: (1) the classical elastohydrodynamic model using resistive force theory and Euler-Bernoulli beam theory, and (2) a novel curve evolution incorporating effects of linear viscoelasticity. We mention our recent PDE results on these models and highlight how this analysis can help to understand undulatory swimming at low Reynolds number. This includes the development of a novel numerical method to simulate inextensible swimmers.

## [04238] A limiting model for a low Reynolds number swimmer with N passive elastic arms

**Format :** Talk at Waseda University

**Author(s) :** Jessie Levillain (CMAP, Ecole Polytechnique)François Alouges (Centre Borelli, École Normale Supérieure Paris-Saclay)Aline Lefebvre-Lepot (CMAP, École polytechnique)

**Abstract :** We study a simple model of artificial microswimmer, consisting of a rigid extensible arm followed by an  $N$ -mass-spring system.

We further study the limit as the number of springs tends to infinity and the parameters are scaled conveniently, and provide a rigorous proof of the convergence of the discrete model to the continuous one.

Numerical experiments show performances of the displacement in terms of frequency or amplitude of the oscillation of the active arm.

## [05406] Activation processes of flagellated micro-swimmers

**Format :** Online Talk on Zoom

**Author(s) :** Irene Anello (SISSA)Jessie Levillain (CMAP, Ecole Polytechnique)François Alouges (Centre Borelli, Ecole Normale Supérieure Paris-Saclay)Aline Lefebvre-Lepot (CMAP, Ecole Polytechnique)Antonio De Simone (SISSA)

**Abstract :** We study the activation processes of flagellated micro-swimmers investigating microscopic details inside the flagellum.

The flagellum is composed of a structure called axoneme, composed of nine filament pairs along which are disposed force-generating elements called molecular motors.

After describing the biology behind it, we first model these motors individually before introducing a mathematical representation of the whole system.

The aim is to couple this microscopic description with a macroscopic beam equation for flagellated swimmers.

## [02171] Emergent rheotaxis of shape-changing swimmers in Poiseuille flow

**Format :** Talk at Waseda University

**Author(s) :** Benjamin Benjamin Walker (University of Bath)Kenta Ishimoto (Kyoto University)Clement Moreau (RIMS, Kyoto University)Eamonn Gaffney (University of Oxford)Mohit Dalwadi (University College London)

**Abstract :** The complexity of microscale swimming has driven the development of simple, representative models. In this talk, we'll examine an apparently simple model of a swimming cell in a channel and reveal a surprisingly complex dynamics that evolves on three distinct timescales. Through an asymptotic analysis, we'll show how the long-time behaviours of this system can be reduced to the study of a single ordinary differential equation, whose evolution turns out to be remarkably simple.

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00286 (2/2) : 2E @A510 [Chair: Jessie Levillain]

## [03303] Nonlinear dynamics, bifurcations and stability transitions in motion of periodically-actuated micro-swimmers

**Format :** Online Talk on Zoom

**Author(s) :** Yizhar Or (Mechanical Engineering, Technion)

**Abstract :** We study simple models of robotic-like microswimmers with periodic actuation. We start from the well-known Purcell's three-link swimmer model, and modify it in order to add realistic effects of passive elasticity and/or mechanical actuation, rather than kinematic control. We also focus on minimal models of magnetically-actuated microswimmers. We show that the nonlinear dynamics of such models include bifurcations and stability transitions of periodic solutions, which can be analyzed both numerically and analytically using asymptotic methods.

## [05278] Low-Reynolds-number swimming via reinforcement learning

**Format :** Online Talk on Zoom

**Author(s) :** Alan C. H. Tsang (University of Hong Kong) Yangzhe Liu (University of Hong Kong) Zonghao Zou (Cornell University) Ali Gurbuz (Santa Clara University) On Shun Pak (Santa Clara University)

**Abstract :** The application of machine learning methods in the development of microswimmers has garnered significant interest recently. In particular, reinforcement learning has proven to be valuable in empowering microswimmers to learn effective propulsion strategies through their interactions with the environment. In this talk, we will discuss our latest progress in integrating reinforcement learning techniques into the design of smart microswimmers capable of performing complex tasks relevant to their biomedical applications.

## [03505] Controllability of microswimming systems with and without drift

**Format :** Talk at Waseda University

**Author(s) :** Clement Moreau (RIMS, Kyoto University)

**Abstract :** In this talk, I will discuss the controllability properties of microswimmer models, i.e. their capacity to reach a given target, depending on important assumptions such as the way the swimmer's deformation is controlled and its environment. I will focus on the example of a magneto-elastic swimmer to present a result on the local controllability of control-affine systems with a drift.

## [03844] Recent trends in micro-swimming

**Format :** Talk at Waseda University

**Author(s) :** Marta Zoppello (Politecnico di Torino) Marco Morandotti (Politecnico di Torino - P. IVA 00518460019)

**Abstract :** Inertialess hydrodynamics is notorious for its time-reversibility constraint, which leads to the well known "Scallop Theorem". One way to overcome it is to couple two or more micro-swimmer units. In this talk we will show some recent results about the controllability of more than one micro-swimmer immersed in a viscous fluid, highlighting the crucial role of hydrodynamic interaction in achieving it.

# [00289] Nonconvex nonlinear programming: Theory and algorithms

**Session Time & Room :**

00289 (1/2) : 1C (Aug.21, 13:20-15:00) @D501

00289 (2/2) : 1D (Aug.21, 15:30-17:10) @D501

**Type :** Proposal of Minisymposium

**Abstract :** Nonconvex nonlinear programming problems arise extensively in many important applications including machine learning, image processing, etc. This minisymposium intends to present the latest advances on nonconvex nonlinear programming both in theory and in algorithms. The talks will be particularly focused on large scale problems, Lagrangian methods, gradient methods, and stochastic methods.

**Organizer(s) :** Xin-Wei Liu, Yakui Huang

**Classification :** 90C06, 90C30, 65K05

**Minisymposium Program :**

00289 (1/2) : 1C @D501 [Chair: Yakui Huang]

## [02633] A Stochastic Conjugate Gradient Algorithm with Variance Reduction

**Format :** Talk at Waseda University

**Author(s) :** Caixia Kou ( Beijing University of Posts and Telecommunications)

**Abstract :** Stochastic gradient descent methods are popular for large scale optimization but has slow convergence asymptotically due to the inherent variance. To remedy this problem, we firstly propose a new stochastic conjugate gradient algorithm, called SCGA. Besides, developing a new stochastic gradient estimate of unbiasedness with minimized variance, we also present another two stochastic conjugate gradient algorithms. The convergence theory can be established and experiments show the new algorithms have satisfactory numerical performance.

## [01352] Golden ratio Bregman proximal gradient algorithm for nonconvex optimization problems

**Format :** Talk at Waseda University

**Author(s) :** Xue Gao (Hebei University of Technology)Kai Wang (Nanjing University of Science and Technology)

**Abstract :** We focus on solving the nonconvex nonsmooth minimization problem over abstract constraint set, whose objective function is the sum of a proper lower semicontinuous convex function and a smooth nonconvex function, where the differentiable part is freed from the restrictive assumption of global Lipschitz gradient continuity. We design, analyze and test a golden ratio Bregman proximal gradient algorithm (GBPG). The globally convergence of GBPG is proved and numerical simulations demonstrate its feasibility and effectiveness.

## [02076] On the quadratic termination property of the gradient method

**Format :** Talk at Waseda University

**Author(s) :** Yakui Huang (Hebei University of Technology)

**Abstract :** The gradient method is one of the most popular algorithms in solving large scale unconstrained optimization problems. However, most of existing gradient methods do not enjoy the quadratic termination property. In this talk, we will provide a summary account of recent and new results on how to equip gradient methods with the two-dimensional quadratic termination property. Moreover, a new mechanism for the gradient method to achieve three- and higher-dimensional quadratic termination will be presented.

## [03083] A novel augmented Lagrangian and its application in linear programming

**Format :** Talk at Waseda University

**Author(s) :** Xinwei Liu (Hebei University of Technology)

**Abstract :** We introduce a twice differentiable augmented Lagrangian for optimization with general inequality constraints. Our function is a combination of the augmented Lagrangian and the logarithmic-barrier technique, and is a generalization of the Hestenes-Powell augmented Lagrangian. The associated augmented Lagrangian method is proved to have strong global convergence, the capability of rapidly detecting the possible infeasibility, and linear convergence to the KKT point. The preliminary numerical experiments on some small benchmark test problems demonstrate our theoretical results. The application in linear programming shows its superiority.

00289 (2/2) : 1D @D501 [Chair: Mengwei Xu]

## [01520] Sensitivity analysis for value functions with application to bilevel programs

**Format :** Talk at Waseda University

**Author(s) :** Kuang Bai (The Hong Kong Polytechnic University)

**Abstract :** In this talk, we will study sensitivity analysis of value functions and optimality conditions of bilevel programs. First, for the sensitivity analysis, based on a recent work of the speaker on parametric nonlinear programs, we will further study the directional sensitivity analysis of value functions for parametric set-constrained problems, which include many classical problems as special cases and can be nonsmooth and nonconvex. In particular, we will derive sufficient conditions for the directional Lipschitz continuity, formulae of the directional derivative and upper estimates for the directional limiting\Clarke subdifferential of value functions. Finally, based on the recent development on directional constraint qualifications and directional optimality conditions, using the directional differential properties of value functions, we will derive sharp optimality conditions for general bilevel programs.

## [03119] Extrapolated Bregman proximal difference-of-convex(DC) algorithm for structured DC optimization problems

**Format :** Talk at Waseda University

**Author(s) :** Bo Wen (Hebei University of Technology)

**Abstract :** In this talk, we mainly consider a Bregman proximal DC method with extrapolation for solving structured DC optimization problems. We first show different extrapolation strategies to possibly accelerate Bregman proximal DC algorithm, and then we discuss the convergence behavior and convergence rates of the Bregman extrapolated proximal DC algorithms. Finally, some numerical experiments have been conducted to illustrate the theoretical results.

## [03077] Relaxed constant positive linear dependence constraint qualification for disjunctive programs

**Format :** Talk at Waseda University

**Author(s) :** Mengwei Xu (Hebei University of Technology) Jane Ye (University of Victoria)

**Abstract :** The disjunctive program is a class of optimization problems in which the constraint involves a disjunctive set which is the union of finitely many polyhedral convex sets. In this paper, we introduce a notion of the relaxed constant positive linear dependence constraint qualification (RCPLD) for the disjunctive program. Our notion is weaker than the one we introduced for a nonsmooth system which includes an abstract set constraint recently (J. Glob. Optim. 2020) and is still a constraint qualification for a Mordukhovich stationarity condition for the disjunctive program. To obtain the error bound property for the disjunctive program, we introduce the piecewise RCPLD under which the error bound property holds if all inequality constraint functions are subdifferentially regular and the rest of the constraint functions are smooth. We then specialize our results to the ortho-disjunctive program, which includes the mathematical program with equilibrium constraints (MPEC), the mathematical program with vanishing constraints (MPVC) and the mathematical program with switching constraints (MPSC) as special cases. For MPEC, we recover MPEC-RCPLD, a MPEC variant of RCPLD and propose the MPEC piecewise RCPLD to obtain the error bound property. For MPVC, we introduce MPVC-RCPLD as a constraint qualification and the piecewise RCPLD as a sufficient condition for the error bound property. For MPSC, we show that both RCPLD and the piecewise RCPLD coincide and hence it is not only a constraint qualification, but also a sufficient condition for the error bound property.

## [03103] An Oracle Gradient Regularized Newton Method for Quadratic Measurements Regression

**Author(s) :** Jun Fan (Hebei University of Technology)

**Abstract :** Recently, recovering an unknown signal from quadratic measurements has gained popularity because it includes as special cases many interesting applications such as phase retrieval, fusion frame phase retrieval and positive operator-valued measure. In this paper, by employing the least squares approach to reconstruct the signal, we establish the non-asymptotic statistical property showing that the gap between the estimator and the true signal is vanished in the noiseless case and is bounded in the noisy case by an error rate of  $O(\sqrt{p \log(1+2n)/n})$ , where  $n$  and  $p$  are the number of measurements and the dimension of the signal, respectively. We develop a gradient regularized Newton method (GRNM) to solve the least squares problem and prove that it converges to a unique local minimum at a superlinear rate under certain mild conditions. In addition to the deterministic results, GRNM can reconstruct the true signal exactly for the noiseless case and achieve the above error rate with a high probability for the noisy case. Numerical experiments demonstrate the GRNM performs nicely in terms of high order of recovery accuracy, faster computational speed, and strong recovery capability.

## [00294] Machine Learning and Differential Equations

**Session Time & Room :**

00294 (1/2) : 4C (Aug.24, 13:20-15:00) @G401

00294 (2/2) : 4D (Aug.24, 15:30-17:10) @G401

**Type :** Proposal of Minisymposium

**Abstract :** This Minisymposium aims at exploring the multiple relations between Machine Learning and Differential Equations. For one, it is possible to use Machine Learning to learn the solutions of challenging, high-dimensional or parameterized Differential Equations. On the other hand, some network architectures, like ResNet or Fractional-DNN, can be understood as time discretizations of Differential Equations. This interplay of different research directions leads to exciting problem formulations and the opportunity to benefit from the respective expertise.

**Organizer(s)** : Roland Maier, Evelyn Herberg  
**Classification** : 34A25, 49J15, 65N30, 68T07  
**Minisymposium Program** :

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00294 (1/2) : 4C @G401

## [01809] Certified machine learning: Rigorous a posteriori error bounds for physics-informed neural networks

**Author(s)** : Birgit Hillebrecht (SimTech, University of Stuttgart) Benjamin Unger (SimTech, University of Stuttgart)  
**Abstract** : Prediction error quantification has been left out of most methodological investigations of neural networks for both purely data-driven and physics-informed approaches. Beyond statistical investigations and generic a-priori results on the approximation capabilities of neural networks, we present a rigorous upper bound on the prediction error of physics-informed neural networks applied to linear PDEs. Our bound can be calculated without knowing the true solution and using only the characteristic properties of the underlying dynamical system.

## [04004] Control of kinetic collective dynamics by deep neural feedback laws

**Author(s)** : Sara Bicego (Imperial College London) Giacomo Albi (Università degli Studi di Verona) Dante Kalise (Imperial College London)  
**Abstract** : We address how to successfully condition high dimensional multi agent systems towards designed cooperative goals via dynamic optimization. The problem reads as the minimization of a cost functional subject to individual-based dynamics; thus, its solution becomes unfeasible as the number of agents grows. We propose a NN-accelerated Boltzmann scheme for approaching the solution from suboptimality. Under the quasi-invariant limit of binary interactions we approximate the mean field PDE governing the dynamics of the agents' distribution.

## [04705] An Operator-Learning Approach for Computational Fluid Dynamics

**Author(s)** : Viktor Hermann Grimm (University of Cologne) Axel Klawonn (University of Cologne) Alexander Heinlein (Delft University of Technology (TU Delft))  
**Abstract** : We present an operator-learning approach for Computational Fluid Dynamics using Convolutional Neural Networks (CNNs). We aim to approximate the solution operator for the incompressible Navier-Stokes equations in varying geometries using CNNs trained only on the underlying physics. No reference simulations are required for training. We show that our method is able to predict the flow field in various geometries sufficiently accurate and compare its performance to traditional numerical methods.

## [04777] Dynamic Control in Machine Learning: Geometric Interpretation of deep neural networks for Multi-Classification and Universal Approximation.

**Author(s)** : Martin Sebastian Hernandez Salinas (Friedrich-Alexander-Universität Erlangen-Nürnberg) Enrique Zuazua (Friedrich-Alexander-Universität Erlangen-Nürnberg)  
**Abstract** : In this talk, we will present recent results on the interplay between control and Machine Learning. We analyze the Residual Neural Networks architecture and the Multilayer Perceptron with minimal width. Adopting a dynamic control and geometric interpretation of the neural networks, we train them in a constructive manner to solve multi-classification problems and achieve simultaneous controllability. We also derive the so-called universal approximation theorems in  $L^p$  spaces for both architectures.

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00294 (2/2) : 4D @G401

## [05167] Fourier Neural Poisson Reconstruction

**Author(s)** : Aras Bacho (Ludwig-Maximilians-Universität München) Héctor Andrade Loarca (Ludwig-Maximilians-Universität München) Julius Hege (Ludwig-Maximilians-Universität München) Gitta Kutyniok (Ludwig-Maximilians-Universität München)  
**Abstract** : 3D Shape Poisson reconstruction is a method for recovering a 3D mesh from an oriented point cloud by solving the Poisson equation. It is widely used in industrial and academic 3D reconstruction applications, but typically requires a large number of points for a reasonable reconstruction. In this talk, I will present a new approach that utilizes Fourier Neural Operators to improve Poisson reconstruction in the low and middle-sampling regime. This method outperforms existing methods in terms of reconstructing fine details and is also resolution-agnostic. This allows for training the network at lower resolutions with less memory usage and evaluating it at higher resolutions with similar performance with much less data points. Furthermore, we demonstrate that the Poisson reconstruction problem is well-posed on a theoretical level by providing a universal approximation theorem for the Poisson problem with distributional data utilizing the Fourier Neuronal Operator which underpins our practical findings.

## [05373] Adaptive Time Stepping in Deep Neural Networks

**Author(s)** : Harbir Antil (George Mason University) Hugo Diaz (University of Delaware) Evelyn Herberg (University Heidelberg)

**Abstract** : We highlight the common features of optimal control problems with partial differential equations and deep learning problems. Furthermore, we introduce a new variable in the neural network architecture, which can be interpreted as a time step-size. The proposed framework can be applied to any of the existing networks such as ResNet or Fractional-DNN. This framework is shown to help overcome the vanishing and exploding gradient issues. The proposed approach is applied to an ill-posed 3D-Maxwell's equation.

## [00295] Estimation problems over groups

**Session Time & Room :**

00295 (1/3) : 5B (Aug.25, 10:40-12:20) @E604

00295 (2/3) : 5C (Aug.25, 13:20-15:00) @E604

00295 (3/3) : 5D (Aug.25, 15:30-17:10) @E604

**Type** : Proposal of Minisymposium

**Abstract** : We discuss a class of estimation problems that aim for unknown group elements or a signal affected by group actions. Three prominent examples of such problems are synchronization over groups, multireference alignment, and the recovery problem in single-particle cryo-EM. The talks will cover computational and theoretical aspects, including the sample complexity of the problems, constructing group invariant operators, sparsity, recovery strategies, machine learning-based methods, group-robust metrics, data modeling, autocorrelation analysis, and its acceleration techniques, manifold optimization in cryo-EM, synchronization analysis, and more. This mini-symposium is divided into three sections and will host senior and junior researchers as its speakers.

**Organizer(s)** : Yuehaw Khoo, Nir Sharon, Amit Singer

**Classification** : 65Kxx, 70Gxx, 92Cxx, 65Jxx, Computational structural biology, Optimization, Manifold Learning, Algebraic Geometry, Information Theory, Machine Learning, Harmonic Analysis, Signal Processing

**Minisymposium Program :**

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00295 (1/3) : 5B @E604 [Chair: Amit Singer]

## [05122] Vector bundles for alignment and dimensionality reduction

**Author(s)** : Jose Perea (Northeastern University) Luis Scoccia (Northeastern University)

**Abstract** : Vector bundles have rich structure and arise naturally when trying to solve dimensionality reduction and synchronization problems in data science. I will show in this talk how the classical machinery (e.g., classifying maps, characteristic classes, etc) can be adapted to the world of algorithms and noisy data, as well as the insights one can gain.

## [04867] Group-robust metrics

**Format** : Online Talk on Zoom

**Author(s)** : William Leeb (University of Minnesota, Twin Cities)

**Abstract** : This talk will describe a family of metrics between functions. These metrics are provably robust to a large class of perturbations of the inputs, including the group of integral-preserving reparameterizations; they are also robust to additive noise, and can be evaluated rapidly. Their theoretical properties will be illustrated by numerical experiments.

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00295 (2/3) : 5C @E604 [Chair: Nir Sharon]

## [04814] The sample complexity of multireference alignment and cryo-EM

**Format** : Talk at Waseda University

**Author(s)** : Tamir Bendory (Tel Aviv University)

**Abstract** : The problem of multi-reference alignment (MRA) involves retrieving a signal from multiple copies that have been corrupted by noise and transformed by a random group element. MRA is of particular interest in the context of single-particle cryo-electron microscopy (cryo-EM), a prominent technique used to reconstruct biological molecular structures. During this talk, I will examine the sample complexity of both the MRA and cryo-EM models using tools from representation theory, sparse coding, and generative models.

## [04753] Autocorrelation analysis for cryo-EM with sparsity constraints

**Format :** Talk at Waseda University

**Author(s) :** Tamir Bendory (Tel Aviv University)Yuehaw Khoo (The University of Chicago)Joe Kileel (UT Austin)Oscar Mickelin (Princeton University)Amit Singer (Princeton University)

**Abstract :** This work presents new results for the method of moments applied to cryo-electron microscopy. We prove that autocorrelations of noisy tomographic projection images can reconstruct molecular structures that are modeled as sparse sums of Gaussians. This significantly reduces the sample complexity of the problem, compared to previous results. Additionally, we detail a practical ab initio reconstruction algorithm using tools adapted from crystallographic phase retrieval.

00295 (3/3) : 5D @E604 [Chair: Yuehaw Khoo]

## [03118] Optimal Spectral Methods for Synchronization Problems

**Format :** Talk at Waseda University

**Author(s) :** Anderson Ye Zhang (University of Pennsylvania)

**Abstract :** We study the performance of spectral methods for synchronization problems with additive Gaussian noises and incomplete data. Spectral methods refer to algorithms that use the leading eigenvectors of the data matrix followed by a normalization step. (1) For phase synchronization and orthogonal group synchronization, we prove that they achieve the minimax lower bound of the problem with a matching leading constant under a squared  $\ell_2$  loss. This shows that the spectral method has the same performance as more sophisticated procedures including MLE, generalized power method, and SDP when consistent parameter estimation is possible. (2) For permutation synchronization, we propose a novel spectral method that overcomes a crucial limitation of existing ones and has improved numerical performance. We further show the proposed method is statistically optimal with an exponentially small error that matches the minimax rate.

## [05181] Orthogonal Matrix Retrieval with Spatial Consensus for 3D Unknown-View Tomography

**Format :** Talk at Waseda University

**Author(s) :** Shuai Huang (Emory University)Mona Zehni (University of Illinois at Urbana-Champaign)Ivan Dokmanic (University of Basel)Zhizhen Zhao (University of Illinois at Urbana Champaign)

**Abstract :** A line of work starting with Kam (1980) employs the method of moments (MoM) with rotation-invariant features to reconstruct a 3D density map from its 2D tomographic projections at unknown, random orientations, assuming that the orientations are uniformly distributed. This line of work includes the recent orthogonal matrix retrieval approaches. In this talk, we extend the previous approaches and propose to jointly recover the density map and the orthogonal matrices by imposing spatial nonnegativity constraint.

# [00296] Recent advances on two-phase flows, fluid-structure interactions, and interface problems

**Session Time & Room :**

00296 (1/3) : 1C (Aug.21, 13:20-15:00) @E701

00296 (2/3) : 1D (Aug.21, 15:30-17:10) @E701

00296 (3/3) : 1E (Aug.21, 17:40-19:20) @E701

**Type :** Proposal of Minisymposium

**Abstract :** This mini-symposium for ICIAM2023 concerns different important topics such as mathematical modeling, theoretical analysis, and numerical methods. An important goal of this workshop is to foster collaboration between mathematicians, computational scientists, and engineers.

Applications include classic interface problems, Newtonian and non-Newtonian fluids, fluid and porous media, or viscoelastic, or poroelastic media couplings, finite element, finite volume, and finite differences or other numerical methods. Wellposedness of mathematical models and so on. The nature of this workshop will be mathematics centered with multi-disciplinary and multi-physics applications.

**Organizer(s) :** Juan Ruiz-Alvarez, Zhiyue Zhang

part\_1

**Classification :** 65M06, 65M60, 76D05, 76T99, 35R35**Minisymposium Program :**

00296 (1/3) : 1C @E701 [Chair: Zhiyue Zhang]

## [02815] High Order Compact Finite Difference Schemes for Helmholtz Interface Problem

**Format :** Talk at Waseda University**Author(s) :** Bin Han (University of Alberta)Qiwei Feng (University of Alberta)Michelle Michelle (Purdue University)Yau Shu Wong (University of Alberta)**Abstract :** The Helmholtz equation is numerically challenging to solve, due to highly oscillating solutions and ill-conditioned huge matrices. Introducing Dirac-Assisted-Tree DAT method and high-order compact FDMs, we can handle 1D-heterogeneous and special 2D-Helmholtz interface problem with large wavenumbers by only solving small linear systems. We present 5th-order compact FDMs for 2D-Helmholtz interface problem with discontinuous wavenumbers and reduced pollution effect. Numerical experiments demonstrate effectiveness and superior performance of our proposed methods for Helmholtz interface problem.

## [03418] Cubic Hermite splines plus correction terms: a way of adaption to the presence of singularities

**Format :** Talk at Waseda University**Author(s) :** Juan Ruiz-Alvarez (Universidad Politecnica de Cartagena)Zhilin Li (North Carolina State University)Sergio Amat (Universidad Politécnica de Cartagena)Juan Carlos Trillo (Universidad Politécnica de Cartagena)Concepción Solano (Universidad Politécnica de Cartagena)**Abstract :** Hermite interpolation is classically used to reconstruct smooth data when the function and its derivatives are available at certain nodes. If derivatives are not available, it is easy to set a system of equations imposing some regularity conditions at the data nodes in order to obtain them. This process leads to the construction of a Hermite spline. The problem of the described Hermite splines is that the accuracy is lost if the data contains singularities. The consequence is the appearance of oscillations, if there is a jump discontinuity in the function, that globally affects the accuracy of the spline, or the smearing of singularities, if the discontinuities are in the derivatives of the function. This work is devoted to the construction and analysis of a new technique that allows for the computation of accurate derivatives of a function close to singularities using a Hermite spline. The idea is inspired in the immersed interface method (IIM) and aims to correct the system of equations of the spline in order to attain the desired accuracy even close to the singularities. Once we have computed the derivatives with enough accuracy, a correction term is added to the Hermite spline in the intervals that contain a singularity. The aim is to reconstruct piecewise smooth functions with  $O(h^4)$  accuracy even close to the singularities. The process of adaption requires some knowledge about the position of the singularity and the values of the function and its derivatives at the singularity. The whole process can be used as a post-processing, where a correction term is added to the classical cubic Hermite spline. Proofs for the accuracy and regularity of the corrected spline and its derivatives are given. We also analyse the mechanism that eliminates the Gibbs phenomenon close to jump discontinuities in the function. The numerical experiments presented confirm the theoretical results obtained.

## [02836] Difference Finite Element Method for 3D Steady Navier-Stokes Equations

**Format :** Talk at Waseda University**Author(s) :** Xinlong Feng (Xinjiang University)**Abstract :** In this work, a difference finite element (DFE) method for the 3D steady Navier-Stokes (N-S) equations is presented. This new method consists of transmitting the FE solution of 3D steady N-S equations into a series of the FE solutions of 2D steady Oseen iterative equations, which are solved by using the finite element pair (P1b,P1b,P1)×P1 satisfying the discrete inf-sup condition in a 2D domain  $\omega$ . In addition, we use finite element pair ((P1b,P1b,P1)×P1)×(P1×P0) to solve 3D steady Oseen iterative equations, where the pair satisfies the discrete inf-sup condition in a 3D domain  $\Omega$  under the quasi-uniform mesh condition. To overcome the difficulty of nonlinearity, we apply the Oseen iterative method and present the weak formulation of the DFE method for solving 3D steady Oseen iterative equations. Moreover, we provide the existence and uniqueness of the DFE solutions of 3D steady Oseen iterative equations and deduce the first order convergence with respect to the discrete step parameter of the DFE solutions to the exact solution of 3D steady N-S equations. Finally, numerical tests are presented to show the accuracy and effectiveness of the proposed method.

## [03698] Finite difference method on staggered grids for Stokes-Biot problems

**Format :** Online Talk on Zoom

**Author(s) :** Hongxing Rui (Shandong University)

**Abstract :** In this talk, we will present a looking-free finite difference method based on staggered grids for coupled Stokes-Biot problems. The model problems are used to describe Stokes fluid coupled with a poroelastic flow with a interface. The construction of the finite difference schemes, analysis for the existence and uniqueness of the approximation solutions, superconvergence will be presented. Numerical experiments are presented to confirm the theoretical results. Then we will present a semi-decoupled scheme for the Stokes-Biot system, where the displacement of structure is split from the whole system using the time-lagging scheme. We will also present some ongoing works on coupled problem briefly.

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00296 (2/3) : 1D @E701 [Chair: Juan Ruiz-Alvarez]

## [05336] Value function approximation of PDEs

**Format :** Talk at Waseda University

**Author(s) :** Kazufumi Ito (North Carolina State University)

**Abstract :** \title{\bf Value function approximation of PDEs}\\ \author{Kazufumi Ito\thanks{Department of Mathematics, North Carolina State University, USA}}\\ \\ \noindent {\bf Abstract} In this paper we discuss a value function approximation of a general class of nonlinear system of parabolic equations. Our approach is based on the backward stochastic differential equations of nonlinear expectation. The approach uses the discrete time dynamic programming formulation of the value function update. It results in an operator splitting of the diffusion term and a semi-implicit method for the nonlinear hyperbolic term. It is very easy to implemented and provides an accurate value function approximation. We apply the method several applications including elliptic interface problems, conservation laws and Navier-Stokes equations. We analyze the stability and convergence of the proposed method. Numerical results are presented to demonstrate the applicability

## [03699] A hybrid asymptotic and augmented compact FVM for degenerate interface problem with extreme conditions

**Format :** Talk at Waseda University

**Author(s) :** Zhiyue Zhang (Nanjing Normal University)

**Abstract :** An accurate and efficient numerical method has been proposed for degenerate interface problem with extreme conditions such as very big jump ratio, coefficient blow-up and geometric singularity interface . The scheme combines Puiseux series asymptotic technique with augmented fourth order compact finite volume method for the problem. Error estimates are obtained. Numerical examples confirm the theoretical analysis and efficiency of the method. We also apply this method for solving time dependent problems and 2D problems.

## [03531] A fast front-tracking approach for a temporal multiscale blood flow problem

**Format :** Talk at Waseda University

**Author(s) :** Ping Lin (University of Dundee)Zhenlin Guo (Beijing Computational Science Research Center)

**Abstract :** We consider a blood flow problem (fast system) coupled with a slow plaque growth with memory effect (slow system) at the artery wall. We construct an auxiliary temporal periodic problem and an effective time-average equation to approximate the original problem and analyze the approximation error of the corresponding PDE system, where the front-tracking technique is used to update the moving boundary. An effective multiscale method is then designed and its approximation error is analysed.

## [03479] An Energy Stable Immersed Boundary Method for Deformable Membrane Problem with Non-uniform Density and Viscosity

**Format :** Online Talk on Zoom

**Author(s) :** Dongdong He (The Chinese University of Hong Kong, Shenzhen)Qinghe Wang (The Chinese University of Hong Kong, Shenzhen)Mingyang Pan (Hebei University of Technology)Yu-Hau Tseng (Kaohsiung University)

**Abstract :** Membrane problems commonly encountered in engineering and biological applications involve large deformations and complex configurations. Immersed boundary method, formulated by the fluid equations in which the fluid-structure interaction is described in terms of the Dirac function, is one of the most powerful tools to simulate such problems. However, the IB method suffers from severe time step restrictions to maintain stability if the discretization part\_1

lacks conservation of energy, especially for two-phase flows. In this paper, we develop an energy stable IB method for solving deformable membrane problems with non-uniform density and viscosity. Unlike the classic IB formulation, the evolution of membrane, including elastic tension and bending force, is controlled by its tangent angle and arc length. After minor modifications, it is shown that the model satisfies the continuous energy law. Thus, for the reformulated model, we proposed an implicit unconditionally energy stable scheme, where the energy of the scheme is proved to be dissipative. The resultant system is solved iteratively and the numerical results show that the proposed scheme is energy stable and capable of predicting the dynamics of extensible and inextensible interface problems with non-uniform density and viscosity.

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00296 (3/3) : 1E @E701

## [00297] Wave scattering problems: numerical methods with applications

**Session Time & Room :**

00297 (1/3) : 1E (Aug.21, 17:40-19:20) @F310

00297 (2/3) : 2C (Aug.22, 13:20-15:00) @F310

00297 (3/3) : 2D (Aug.22, 15:30-17:10) @F310

**Type :** Proposal of Minisymposium

**Abstract :** Wave scattering problems in acoustics, elastodynamics and electromagnetics are important in a large number of applications wherein challenging mathematical and numerical issues require sophisticated methods and techniques to resolve. The study of numerical methods for solving wave scattering problems has been heavily focused by researchers in both mathematical and engineering committees. This symposium devotes to combining experts from different countries and discussing some latest advances in computational modelling and simulation of complex wave phenomena with their application to real-world problems.

**Organizer(s) :** Wangtao Lu, Tao Yin

**Classification :** 35L05, 65Nxx, 78Mxx

**Minisymposium Program :**

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00297 (1/3) : 1E @F310 [Chair: Wangtao Lu]

## [02173] Fast butterfly compressed Hadamard-Babich integrators for Helmholtz equations

**Format :** Talk at Waseda University

**Author(s) :** Jianliang Qian (Michigan State University)Yang Liu (Lawrence Berkeley National Laboratory)

**Abstract :** We present a butterfly-compressed representation of the Hadamard-Babich (HB) ansatz for the Green's function of the high-frequency Helmholtz equation in smooth inhomogeneous media. The proposed scheme can accurately model wave propagation in 2D domains with 640 wavelengths per direction and in 3D domains with 54 wavelengths per direction {on a state-the-art supercomputer at Lawrence Berkeley National Laboratory}.

## [03005] Inverse wave-number dependent source problems

**Format :** Talk at Waseda University

**Author(s) :** Guanghui Hu (Nankai University, Tianjin, China)

**Abstract :** We consider an inverse problem for imaging the support of a wave-number-dependent source function. The source function is given by the Fourier transform of some time-dependent source with a priori given radiating period. Using the multi-frequency far-field data at a fixed observation direction, we provide a necessary and sufficient criterion for characterizing the smallest strip containing the support and perpendicular to the observation direction.

## [04115] The PML-method for a scattering problem for a local perturbation of an open periodic waveguide

**Format :** Talk at Waseda University

**Author(s) :** Andreas Kirsch (Karlsruher Institut für Technologie)Ruming Zhang (Technische Universität Berlin)

**Abstract :** In this talk, we study the convergence of the PML method to approximate wave propagating in an open periodic waveguide. Different from the scattering problem with periodic surfaces, the existence of propagating modes

makes things challenging. We apply a complex contour integral method to deal with the difficulty. Finally an exponential convergence of the PML method is proved.

## [03704] A PML method for signal-propagation problems in axon

**Format :** Talk at Waseda University

**Author(s) :** Xue Jiang (Beijing University of Technology)maohui lyu (Chinese Academy of Sciences)Tao Yin (Chinese Academy of Sciences)Weiying Zheng (Chinese Academy of Sciences)

**Abstract :** This talk concerns the modelling of signal propagations in myelinated axons to characterize the functions of the myelin sheath in the neural structure. We derive a two-dimensional neural-signaling model in cylindrical coordinates from the time-harmonic Maxwell's equations. The well-posedness of model is established. Using the PML method, we propose an approximate problem. The well-posedness of the PML problem and the exponential convergence of the approximate solution to the exact solution are established.

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00297 (2/3) : 2C @F310 [Chair: Tao Yin]

## [01969] Frequency-time Green function acceleration for simulation, optimization and design

**Format :** Talk at Waseda University

**Author(s) :** Oscar P Bruno (Caltech)

**Abstract :** We present a novel "Interpolated Factored Green Function" method (IFGF), including a massively parallel implementation, for the accelerated evaluation of the integral operators in scattering theory and other areas. The IFGF algorithm runs on a small memory footprint, and it is better suited than other methods for efficient distributed-memory parallelization. A variety of applications will be mentioned, including frequency- and time-domain scattering in interior and exterior domains, atmospheric propagation and metamaterial design.

## [03041] Analysis of scattering matrix algorithm

**Format :** Talk at Waseda University

**Author(s) :** Andreas Rathsfeld (Weierstrass Institute for Applied Analysis and Stochastics, Berlin)

**Abstract :** The scattering matrix algorithm is a popular numerical method for the diffraction of optical waves by periodic surfaces. The computational domain is divided into horizontal slices and, by a clever recursion, an approximated operator, mapping incoming into outgoing waves, is obtained. Combining this with numerical schemes inside the slices, methods like RCWA and FMM have been designed. The key for the analysis is the scattering problem with special radiation conditions for inhomogeneous cover materials.

## [04576] On the coupling schemes of finite element and boundary integral equation methods solving the acoustic/elastic scattering problems

**Format :** Talk at Waseda University

**Author(s) :** Liwei Xu (University of Electronic Science and Technology of China)

**Abstract :** In this talk, we introduce two coupling schemes of finite element and boundary integral equation methods solving the acoustic/elastic scattering problems. The first one is the coupling of finite element and Fourier series based boundary integral solving the exterior time-harmonic elastic scattering problem. The second is the coupling of discontinuous Galerkin finite element and boundary integral equations solving the fluid-structure interaction problem. Well-posedness of the approximate problems, analysis on the accuracy and stability of numerical schemes, and numerical results will be presented.

## [03004] Fast multipole method in layered media: from Helmholtz to Maxwell's equations

**Format :** Talk at Waseda University

**Author(s) :** Bo Wang (LCSM(MOE), School of Mathematics and Statistics, Hunan Normal University, Changsha, Hunan, 410081, P. R. China.)

**Abstract :** In this talk, a fast multipole method (FMM) for the dyadic Green's function of Maxwell's equations in layered isotropic media is presented. As in the homogeneous media, layered dyadic Green's function (LDGF) of Maxwell's equation is shown closely related to the Green's function of Helmholtz equation in layered media. Actually, there are only two essential components in the LDGF. By following the theory developed for the Green's function of Helmholtz equation, we derive multipole expansions (MEs) and local expansions (LEs) as well as the multipole-to-local translation

(M2L) operators for all the reaction field components of the LDGF. Then, the FMMs for the LDGF is implemented with the target particles and equivalent polarization sources associated with the reaction field components. Numerical results validate the fast convergence of the MEs and the O(N) complexity of the FMM for N particle problem in 3-D layered media.

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00297 (3/3) : 2D @F310 [Chair: Liwei Xu]

## [03722] Dirac points for the honeycomb lattice with impenetrable obstacles

**Format :** Online Talk on Zoom

**Author(s) :** Junshan Lin (Auburn University)

**Abstract :** Dirac points are special vertices in the band structure when two bands of the spectrum for the operator touch in a linear conical fashion, and their investigations play an important role in the design of novel topological materials. In this talk, I will discuss Dirac points for the honeycomb lattice with impenetrable obstacles arranged periodically in a homogeneous medium. I will discuss both the Dirichlet and Neumann eigenvalue problems and prove the existence of Dirac points for both eigenvalue problems at crossing of the lower band surfaces as well as higher band surfaces. In addition, quantitative analysis for the eigenvalues and the slopes of two conical dispersion surfaces near each Dirac point will be presented by a combination of the layer potential technique and asymptotic analysis.

## [03675] Electronic Structure of Incommensurate 2D Heterostructures with Mechanical Relaxation

**Format :** Online Talk on Zoom

**Author(s) :** Daniel Massatt (Louisiana State University)

**Abstract :** Momentum space transformations for incommensurate 2D electronic structure calculations are fundamental for reducing computational cost and for representing electronic structure data in a more physically motivating format, as exemplified in the Bistritzer-MacDonald model. However, these transformations can be difficult to implement in more complex systems such as when mechanical relaxation patterns are present. In this work, we aim for two objectives. Firstly, we strive to simplify the understanding and implementation of this transformation by rigorously writing the transformations between the four relevant spaces, which we denote real space, configuration space, momentum space, and reciprocal space. This provides a straight-forward algorithm for writing the complex momentum space model from the original real space model. Secondly, we implement this for twisted bilayer graphene with mechanical relaxation affects included. We also analyze the convergence rates of the approximations, and show the tight-binding coupling range increases for smaller relative twists between layers, demonstrating that the 3-nearest neighbor coupling of the Bistritzer-MacDonald model is insufficient when mechanical relaxation is included for very small angles. We quantify this and verify with numerical simulation.

## [03832] Structural Symmetry and Fabry-Perot Bound States in the Continuum: A Numerical Study

**Format :** Talk at Waseda University

**Author(s) :** Zitao MAI (City University of Hong Kong) Ya Yan LU (City University of Hong Kong)

**Abstract :** Fabry-Perot BIC is a special type of BIC occurs in systems with two parallel identical structures acting as ideal mirrors. Similar phenomena may arise in two-layer periodic dielectric structures by tuning different parameters such as the spacing between two layers. In our study, structures with different symmetry properties are used to verify the existence of Fabry-Perot BIC, and the minimum number of tuning parameters required is also examined.

## [00304] Phase transition and control of PDE models in applied sciences

**Session Time & Room :** 4D (Aug.24, 15:30-17:10) @G801

**Type :** Proposal of Minisymposium

**Abstract :** The minisymposium aims to discuss recent developments and applications on phase transition and control for partial differential equations, abbreviated as PDEs, in applied sciences, such as biology, material sciences, engineering and so on.

Partial differential equations are important tools to model and study the various phenomena in applied sciences. The models with phase transition and control issues give rise to a great deal of challenging problems both in theoretical and numerical studies. The sessions focus on the seminal and extensive works in phase transition, boundary stabilization, optimal control of PDE models, such as Keller-Segel model, multi species BGK models, and aggregation models.

**Organizer(s) :** Jie Du, Hui Yu

part\_1

**Classification :** 35Qxx, 65Mxx, 92Bxx**Minisymposium Program :**

00304 (1/1) : 4D @G801

**[01375] Crowd pressure and turbulence in crowd disasters****Format :** Talk at Waseda University**Author(s) :** Liangze Yang (Yanqi Lake Beijing Institute of Mathematical Sciences and Applications)**Abstract :** In this study, a mixed-type continuum model for multidirectional pedestrian flow was developed that explicitly considers the different movement characteristics of pedestrians under different situations: laminar flow in a low-density system and turbulent flow in a high-density system. In addition to the phase transition, the proposed model can reveal the effects of both force chains and panic sentiment, which are commonly observed phenomena during crowd disasters, by estimating the aggregated pushing pressure.**[01721] Traceability of Water Pollution governed by an Inverse Source****Problem****Format :** Talk at Waseda University**Author(s) :** Shenwen Yu (Yau Mathematical Sciences Center, Tsinghua University)Lingyun Qiu (Yau Mathematical Sciences Center, Tsinghua University)Zhongjing Wang (Department of Hydraulic Engineering, Tsinghua University)Hui Yu (Yau Mathematical Sciences Center, Tsinghua University)**Abstract :** We aim to find the time-dependent source term in the diffusion equation from the boundary measurement. Based on the idea of dynamic complex geometrical optics (CGO) solutions, we analyze a variational formulation of the inverse source problem and prove the uniqueness and stability result. A two-step reconstruction algorithm is proposed, which first recovers the locations of the point sources, and then the emission concentration functions. Some numerical experiments on simulated data are conducted.**[03877] A Cucker-Smale inspired deterministic Mean Field Game with velocity interactions****Format :** Talk at Waseda University**Author(s) :** Woojoo Shim (Kyungpook National University)Filippo Santambrogio (Université Claude Bernard - Lyon 1)**Abstract :** In this talk, I would like to introduce a mean field game model for pedestrians moving in a given domain and choosing their trajectories so as to minimize a cost including a penalization on the difference between their own velocity and that of the other agents they meet. During the talk, we will study the existence of an equilibrium in a Lagrangian setting using its variational structure and then study its properties and regularity.**[05554] Provable convergence of blow-up time of numerical approximations for a class of convection-diffusion equations****Format :** Online Talk on Zoom**Author(s) :** Yang Yang (Michigan Technological University)**Abstract :** In this talk, we investigate the numerical algorithms to capture the blow-up time for a class of convection-diffusion equations with blow-up solutions, such as the chemotaxis model. The blow-up time is difficult to capture since we cannot distinguish whether the blow-up is physical or is due to the instability. We propose two ways to define the numerical blow-up time and prove the convergence to the exact one.**[00305] Computational Modeling on Biomedical Diseases****Session Time & Room :**

00305 (1/2) : 4E (Aug.24, 17:40-19:20) @A511

00305 (2/2) : 5B (Aug.25, 10:40-12:20) @A511

**Type :** Proposal of Minisymposium

**Abstract :** Several studies have demonstrated that mathematical and computational data analysis models are required to obtain a systematic understanding of the diseases and find effective treatments. As a result, many mathematical models using both stochastic and deterministic methods have been developed to study the evolutionary processes of the diseases' initiation and progression. Some of the results of these computational models were used to predict the outcome of various drugs to obtain optimal treatment strategies. This mini-symposium will bring together scientists who are interested in the mathematical modeling of different biomedical diseases, including COVID-19, AIDS, TB, cancer, etc.

**Organizer(s) :** Wenrui Hao, Wing-Cheong Lo, Leli Shahriyari

**Classification :** 92-10, 92B05, 92C50

**Minisymposium Program :**

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00305 (1/2) : 4E @A511 [Chair: Wing-Cheong Lo]

### [00317] Role of senescent tumor cells and macrophages in building a cytokine shield in the tumor microenvironment: mathematical modeling

**Format :** Talk at Waseda University

**Author(s) :** Yangjin Kim (Konkuk University)Junho Lee (B)Chaeyoung Lee (Korea University)Sean Lawler (Brown University)

**Abstract :** Cellular senescence can induce dual effects (promotion or inhibition) on cancer progression. While immune cells naturally respond and migrate toward various chemotactic sources from the tumor mass, various factors including senescent tumor cells (STCs) in the tumor microenvironment (TME) may affect this chemotactic movement. In this work, we investigate the mutual interactions between the tumor cells and the immune cells (T cells and macrophages) that either inhibit or facilitate tumor growth by developing a mathematical model that consists of taxis-reaction-diffusion equations and receptor kinetics for the key players in the interaction network. We first apply a mathematical model to a transwell Boyden chamber invasion assay used in the experiments to illustrate that STCs can play a pivotal role in negating immune attack through tight regulation of intra- and extra-cellular signaling molecules. In particular, we show that senescent tumor cells in cell cycle arrest can block intratumoral infiltration of CD8+ T cells by secreting a high level of CXCL12, which leads to significant reduction its receptors, CXCR4, on T cells, and thus impaired chemotaxis. Macrophages also play an important role in mediating or inhibiting given signaling pathways between different cells in TME. The predictions of nonlinear responses to CXCL12 were in good agreement with experimental data. We tested several hypotheses on immune-tumor interactions under various biophysical- and biochemical- conditions in the tumor microenvironment and developed new concepts for anti-tumor strategies targeting senescence induced immune impairment.

### [00373] Patch formation driven by stochastic effects of interaction between viruses and defective interfering particles

**Format :** Talk at Waseda University

**Author(s) :** Qiantong Liang (City University of Hong Kong)Wing-Cheong Lo (City University of Hong Kong)

**Abstract :** We develop a model with a new hybrid method to study the spatial-temporal dynamics of viruses and DIPs co-infections within hosts. We present two scenarios of virus production and compare the results from deterministic and stochastic models to demonstrate how the stochastic effect is involved in the spatial dynamics of virus transmission. Our simulations demonstrate that DIPs can slow down the growth of virus particles and make the spread of virus more patchy.

### [01228] Modeling about prediction and improvement of therapeutic efficacy of immune checkpoint inhibitors

**Format :** Talk at Waseda University

**Author(s) :** Xiulan Lai (Renmin University of China)

**Abstract :** Immune checkpoint inhibitors have been shown to be highly successful against some solid metastatic malignancies, but the overall patient response rate is limited due to the interpatient heterogeneity. In this project, we explored the effect of favorable and unfavorable gut bacteria on the therapeutic efficacy of anti-PD-1 against cancer by modeling the tumor-immune-gut microbiome interactions, and further examined the predictive markers of responders and non-responders to anti-PD-1. The dynamics alteration of PD-L1 expression status during cancer evolution and treatment are also obstacles for PD-1/PD-L1 inhibitors. We established a comprehensive modeling and computational framework for estimating the dynamic alternation of PD-L1 heterogeneity during cancer progression and treatment, and predicting the overall survival of patients.

**[01252] Travelling waves of a new glioma invasion model.****Format :** Talk at Waseda University**Author(s) :** Ryan Thiessen (University of Alberta)**Abstract :** Recently a detailed study of in-vivo glioma invasion patterns in the healthy brain tissue of living mice shows that specialized cancer cells build a network similar to a healthy brain neuronal network. We develop a model for this new phenomenon via a kinetic formulation. After making some simplifying assumptions, we arrive at a reaction-diffusion model. In this talk, I will explore travelling waves for the simplified new glioblastoma model.

00305 (2/2) : 5B @A511 [Chair: Wenrui Hao]

**[01194] The role of the autoregulation mechanism in hypertension and hypotension in humans****Format :** Talk at Waseda University**Author(s) :** Radu C Cascaval (University of Colorado Colorado Springs)**Abstract :** We present a nonlinear model for the propagation of the pressure and flow velocity waves in the human cardiovascular system, including deep learning tools with available physiological data. This model is used for understanding the system-level dynamics of the pressure and flow rates. This time-domain analysis is best to describe time-dependent controls, collectively known as the autoregulation mechanism. We discuss an application of our model to the study of the hypertension and hypotension.**[01215] Collaborative research toward data driven mathematical modeling of cancer to arrive at effective treatments****Format :** Talk at Waseda University**Author(s) :** Leili Shahriyari (University of Massachusetts Amherst)**Abstract :** Cancer is a complex disease with many unknown features. The evolution of tumors greatly depends on the interaction network among different cell types, including immune cells and cancer cells in the tumor. To overcome some of the outstanding challenges of mathematical modeling of cancer, we have utilized and integrated several computational techniques. Importantly, in collaboration with scientists with diverse backgrounds, we have used patients' data and rich spatio-temporal mouse data to develop data-driven mathematical models for tumors' progression. We believe a collaborative model for conducting research and sharing resources, including codes, data, and results would improve our chances to arrive at more effective treatments and ultimately eliminate cancer as a major health problem for this and future generations. In this talk, I will provide an overview of some of our recent collaborative works and outline several outstanding challenges and possible next steps to address them.**[01334] Phase-field model of mechanical stability of blood clot****Format :** Online Talk on Zoom**Author(s) :** Zhiliang Xu (University of Notre Dame)**Abstract :** Deformation and detachment of blood clot (thrombus) under different flow conditions are studied. The fibrin and activated platelets are assumed to concentrate in the core of a thrombus and less-activated platelets are assumed to concentrate in the shell region near the boundary of a thrombus. Interactions among different components are simulated by using Cahn-Hilliard type systems of equations. The macroscopic motion of fluid is described by incompressible Navier-Stokes equations with terms representing viscos, elastic and phase interaction forces as well as porous media drag force. Model simulations predict that the permeability and porosity  $\phi$  of the shell region are shown to effect the stablility of the blood clot. The stablity of the red blood cell cavity at different position in the blood clot are also illustrated.**[00306] Mathematical approaches to nonlinear phenomena with singularities****Session Time & Room :**

00306 (1/3) : 4C (Aug.24, 13:20-15:00) @G601

00306 (2/3) : 4D (Aug.24, 15:30-17:10) @G601

00306 (3/3) : 4E (Aug.24, 17:40-19:20) @G601

**Type :** Proposal of Minisymposium

**Abstract :** In the advanced sciences and technologies, singularity has been one of characteristic keywords of complex and dynamic nonlinear phenomena, such as phase transitions, crystallization processes, image denoising processes, and so on. Also, in recent years, the theoretical/numerical methods to deal with such singularity have been developed by a lot of researchers, from various viewpoints. The objective of this mini-symposium is to let wide range of experts of this field meet together, and to exchange the latest hot topics on the mathematical models of nonlinear phenomena, such as solvability, regularities, stability, optimizations, and so on.

**Organizer(s) :** Ken Shirakawa, Salvador Moll, Hiroshi Watanabe

**Classification :** 35J75, 35K67, 35L81, 49S05, 35R35

**Minisymposium Program :**

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00306 (1/3) : 4C @G601 [Chair: Ken Shirakawa]

## [04427] Crystalline inverse mean curvature flow

**Format :** Talk at Waseda University

**Author(s) :** Marcos Solera Diana (Universidad Autónoma de Madrid/Universitat de València)

**Abstract :** We obtain existence of minimizers for the  $p$ -capacity functional defined with a symmetric anisotropy for  $1 < p < \infty$  and the associated Euler-Lagrange equation. After a change of variables and letting  $p \downarrow 1$  we are led to the existence of solutions to the elliptic PDE associated with the level set formulation of the crystalline inverse mean curvature flow.

## [04365] Pseudo-parabolic model of grain boundary motion coupled with solidification effect

**Format :** Talk at Waseda University

**Author(s) :** Daiki Mizuno (Chiba University)Ken Shirakawa (Chiba University)

**Abstract :** In this talk, we consider a coupled nonlinear system, which consists of an Allen-Cahn type equation and a pseudo-parabolic KWC type system. The system is based on the  $\phi\text{-}\eta\text{-}\theta$  model of grain boundary motion with solidification (cf. RIMS Kokyuroku, 1210, 2001). Under suitable assumptions, the mathematical results concerned with the well-posedness, including open question of uniqueness, and fine-regularity of the solution will be discussed in the Main Theorems of this talk.

## [04655] Elliptic problems involving a Hardy potential

**Format :** Talk at Waseda University

**Author(s) :** Alexis Molino (University of Almeria)

**Abstract :** In this talk we consider different elliptic differential equations with a potential Hardy type singularity in a domain and Dirichlet conditions on the boundary. Specifically, the regularizing effect of lower order terms is revealed, as well as the existence of solutions beyond the well-known Hardy constant.

## [04200] Solvability of a phase-field model of 3D-grain boundary motion

**Format :** Talk at Waseda University

**Author(s) :** Salvador Moll (Universitat de Valencia)Ken Shirakawa (Chiba University)Hiroshi Watanabe (Oita University)

**Abstract :** We consider a phase-field model of 3D-grain boundary motion. The model is based on the three dimensional Kobayashi-Warren model for the dynamics of polycrystals. To formulate our 3D-model, we use a quaternion formulation for the orientation variable.

In this talk, we obtain existence of solutions to the  $L^2$ -gradient descent flow of the constrained energy functional via several approximating problems. Moreover, we also obtain an invariance principle for the orientation variable.

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00306 (2/3) : 4D @G601 [Chair: Hiroshi Watanabe]

## [03754] Variational models for segmentation in non-euclidian settings

**Format :** Talk at Waseda University

**Author(s) :** Salvador Moll (Universitat de Valencia)

**Abstract :** I will present some new results on image segmentation in the general framework of perimeter measure spaces; including the anisotropic case and non-euclidian settings such as random walk spaces or metric graphs.

I will show the linkage between the ROF model for denoising and the two phases piecewise constant segmentation and I will show different applications of the results to nonlocal image segmentation, via discrete weighted graphs, and to multiclass classification on high dimensional spaces.

## [04356] Periodic solution to KWC-type system under dynamic boundary condition

**Format :** Talk at Waseda University

**Author(s) :** Ryota Nakayashiki (Salesian Polytechnic)Ken Shirakawa (Chiba University)

**Abstract :** The aim of this study is to observe the periodic stability for KWC-type system of grain boundary motion under dynamic boundary condition. The KWC-type system is a collective term of PDE model of grain boundary motion (cf. Kobayashi et al, Physica D 140, 2000), which is governed by variable-dependent singular diffusion equation. As one of key-results of the study, we will prove the main theorem concerned with the existence of periodic solution.

## [03968] Cahn-Hilliard equations with forward-backward dynamic boundary condition and non-smooth potentials

**Format :** Talk at Waseda University

**Author(s) :** Pierluigi Colli (Università degli Studi di Pavia)Takeshi Fukao (Ryukoku University)Luca Scarpa (Politecnico di Milano)

**Abstract :** The asymptotic behavior as the coefficient of the surface diffusion acting on the boundary phase variable goes to 0 is investigated. By this analysis we obtain a forward-backward dynamic boundary condition at the limit. We can deal with a general class of potentials having a double-well structure, including the non-smooth double-obstacle potential. We illustrate that the limit problem is well-posed by also proving a continuous dependence estimate

## [04411] Optimal control for shape memory alloys of the simplified Fr'emon model in the one-dimensional case

**Format :** Talk at Waseda University

**Author(s) :** Noriaki Yamazaki (Kanagawa University)Ken Shirakawa (Chiba University)Pierluigi Colli (Università degli Studi di Pavia)M. Hassan Farshbaf-Shaker (Weierstrass Institute for Applied Analysis and Stochastics)

**Abstract :** In this talk, we consider optimal control problems for the one-dimensional Fremond model for shape memory alloys.

Then, we prove the existence of an optimal control that minimizes the cost functional for a nonlinear and nonsmooth state problem. Moreover, we show the necessary condition of the optimal pair by using optimal control problems for approximating systems.

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00306 (3/3) : 4E @G601 [Chair: Salvador Moll]

## [03661] Geometric convergence in regularization of inverse problems

**Format :** Talk at Waseda University

**Author(s) :** Jose A. Iglesias (University of Twente)Gwenael Mercier (University of Vienna)Kristian Bredies (University of Graz)Otmar Scherzer (University of Vienna)

**Abstract :** We present some results bridging classical regularization theory of ill-posed inverse problems and regularity properties of almost-minimizers of the corresponding regularization energies. In the regime of vanishing noise and regularization parameter, we obtain results of convergence in Hausdorff distance of level sets of minimizers (which can be interpreted as objects to be recovered in an imaging context) and uniform  $L^\infty$  bounds. These hold both for the classical total variation, and for some fractional energies.

## [04617] Numerical algorithms for optimization problems of grain boundary motions

**Format :** Talk at Waseda University

**Author(s) :** Shodai Kubota (National Institute of Technology, Miyakonojo College)Ken Shirakawa (Chiba University)Makoto Okumura (Konan University)

**Abstract :** We consider a class of optimal control problems for state problems of one-dimensional systems. Each state problem is associated with the phase-field model of grain boundary motion, proposed by Ryo Kobayashi et al. In this regard, each optimal control problem is prescribed as a minimization problem of a cost. Under suitable assumptions, the convergence of numerical algorithms for optimization problems governed by state systems will be reported as the main theorem of this talk.

## [04370] Temperature optimization problems governed by pseudo-parabolic model of grain boundary motion

**Format :** Talk at Waseda University

**Author(s) :** Ken Shirakawa (Chiba University)Daiki Mizuno (Chiba University)

**Abstract :** In this talk, we consider a class of optimal temperature control problems governed by pseudo-parabolic PDE systems. The PDE systems are based on the KWC-model of grain boundary motion (cf. Kobayashi et al, Physica D, 140, 2000). Under suitable assumptions, we will focus on the Main Theorems, concerned with: the mathematical solvability and parameter dependence of pseudo-parabolic PDE systems and optimal controls; and the first-order necessary optimality conditions for the optimal control problems.

## [04841] On well-posedness of 1-harmonic map flows

**Format :** Online Talk on Zoom

**Author(s) :** Lorenzo Giacomelli (Sapienza University of Rome)Michał Lasica (Institute of Mathematics of the Polish Academy of Sciences)Salvador Moll (Universitat de ValènciaUniversity of Valencia)

**Abstract :** We look at the formal gradient flow of the total variation of a manifold-valued unknown function. After introducing the problem and the state-of-the-art, I will discuss recent results with M. Lasica and S. Moll concerning local/global-in-time well-posedness of Lipschitz solutions and global existence of BV-solutions for one-dimensional domains. Uniqueness, gradient flow structures, and open questions will also be discussed.

# [00307] Advanced Solver for Computational Poromechanics

**Session Time & Room :** 2C (Aug.22, 13:20-15:00) @D404

**Type :** Proposal of Minisymposium

**Abstract :** The numerical simulation of coupled flow and mechanical deformation in porous media is desired in several branches of technology and natural sciences for analyzing experimental data and designing quantitative theories based on mathematical concepts. The fluid-structure interaction is subject to various complexities and multiscale mechanisms. This is due to the mixed or mixed dimensional type of the model equations, nonlinearities in constitutive relations or boundary conditions, functionals used in variational formulations of error control or optimization problems. Recent progress in the design, analysis and application to large-scale problems of robust and efficient solvers for poromechanics is presented by leading experts.

**Organizer(s) :** Markus Bause, Florin A. Radu

**Classification :** 76S05, 65M60, 35M33, 65N55, Poromechanics

**Minisymposium Program :**

00307 (1/1) : 2C @D404 [Chair: Markus Bause]

## [01387] A coupled multi-field model of dynamic poro-elasticity in anisotropic porous media

**Format :** Talk at Waseda University

**Author(s) :** Massimiliano Ferronato (University of Padova)Nico De Marchi (University of Padova)Giovanna Xotta (University of Padova)Valentina Salomoni (University of Padova)

**Abstract :** A fully coupled multi-field model for the dynamic simulation of anisotropic porous materials is presented. The multi-field formulation of the dynamic poro-elastic PDEs is addressed by using inf-sup stable Finite Element spaces and solved in a fully-implicit way. The GMRES convergence of the discrete non-symmetric linearized systems is accelerated by an ad-hoc Multi-Physics Reduction preconditioning technique. A set of dynamic test problems verify the potential and computational efficiency of the proposed numerical model.

## [01468] Space-time finite element multigrid solver for fully dynamic poroelasticity

**Format :** Talk at Waseda University

**Author(s) :** Markus Bause (Helmut Schmidt University Hamburg)Mathias Anselmann (Helmut Schmidt University Hamburg)

**Abstract :** Space-time finite element methods ((STFEMs)) allow the natural construction of higher order discretizations and to achieve accurate results on computationally feasible grids. We present and analyze higher order STFEMs for two-

and multi-field modelling of poroelastic wave propagation studied, for instance, in computational seismology or biomedicine. To solve the arising complex algebraic systems, geometric multigrid preconditioning with local Vanka-type smoother of GMRES iterations is suggested. The STFEMs performance is investigated for three-dimensional test problems.

## [01676] Multiscale Dynamics in Glioblastoma Growth and Spread within the Fibrous Brain Environment

**Format :** Talk at Waseda University

**Author(s) :** Dumitru Trucu (University of Dundee, Division of Mathematics)

**Abstract :** Despite significant recent advancements, the 3D glioblastoma invasion patterns in the brain are still poorly understood. A particular role in the collective migration of the glioblastoma cells is played by the distribution of both major brain fibres and collagen fibres present at the tumour site. To address this aspect, in this talk we present our recent advances in this direction, focusing on our recent 3D multiscale moving-boundary modelling and computational framework development for glioblastoma invasion.

## [01820] Efficient splitting schemes for poromechanics

**Format :** Online Talk on Zoom

**Author(s) :** Florin Adrian Radu (University of Bergen)

**Abstract :** In this work we will present robust and efficient numerical schemes for poromechanics. Monolithic or splitting solvers will be discussed. A special focus will be on non-linear poromechanics models, including soft material poromechanics. Splitting ideas will be combined with L-scheme and Anderson acceleration to design robust and effective numerical schemes. Convergence aspects will be discussed both theoretically and numerically.

## [00309] Population Dynamics in Biology and Medicine

**Session Time & Room :**

00309 (1/4) : 1C (Aug.21, 13:20-15:00) @A601

00309 (2/4) : 1D (Aug.21, 15:30-17:10) @A601

00309 (3/4) : 1E (Aug.21, 17:40-19:20) @A601

00309 (4/4) : 2C (Aug.22, 13:20-15:00) @A601

**Type :** Proposal of Minisymposium

**Abstract :** The mini-symposium covers diverse topics in population dynamics, from the control of insect populations, which are important disease vectors or agricultural pests, to disease spreading and their relationship with the individual immunological status in an ecological ambiance. Different approaches will be discussed in this context, combining techniques from control theory, asymptotic analysis, bifurcation theory, sensitivity analysis, and networks. The group committed to this mini-symposium is heterogeneous, coming from different institutions in North and South America, Europe, and Asia, and well-balanced between women and men researchers.

**Organizer(s) :** Claudia Pio Ferreira, Olga Vasilieva

**Classification :** 92B05

**Minisymposium Program :**

00309 (1/4) : 1C @A601 [Chair: Olga Vasilieva]

## [01291] Exploring the effects of the latent eggs on the efficacy of Wolbachia-carrying release technique

**Format :** Talk at Waseda University

**Author(s) :** Claudia Pio Ferreira (Unesp)

**Abstract :** I will present an ordinary differential system that takes into account the interaction of two populations of mosquito, infected and uninfected with wolbachia. Each population will be split in egg, latent egg, larva and adult stage, but for the infected population no transition to larvae coming through latent egg is possible. Therefore, we will explore the contribution of uninfected eggs coming from the latent stage to the efficacy of wolbachia-aedes release.

## [01943] Mathematical models for practical application of the Sterile Insect Technique

**Format :** Talk at Waseda University

**Author(s) :** Yves Dumont (CIRAD - University of Pretoria)

**Abstract :** Sterile Insect Technique-SIT is an autocidal control method used against Pests and Vectors. While conceptually very simple, it can be difficult to set up in the field. That is why, it is sometimes successful, and sometimes not. We show that modeling, analysis and simulations can be helpful to limit the risk of failure in SIT feasibility programs. We present some results obtained against Aedes albopictus and Bactrocera dorsalis in Réunion island, a French overseas department.

## [01092] A generalized next generation method for the effective reproduction number

**Format :** Talk at Waseda University

**Author(s) :** Suani Tavares Rubim de Pinho (Universidade Federal da Bahia) Daniel Cardoso Pereira Jorge (Universidade Estadual Paulista) Julianne Fonseca Oliveira (CIDACS - Fundação Oswaldo Cruz) José Garcia Vivas Miranda (Universidade Federal da Bahia) Roberto Fernandes Silva Andrade (Universidade Federal da Bahia)

**Abstract :** The effective reproduction number  $R(t)$  plays a key role in the study of infectious diseases, indicating the current average number of new infections caused by an infected individual. In this work, we present a generalization of next generation method, leading to expressions of  $R(t)$  and generation interval distributions, within and between model sub-compartments, provided by an arbitrary compartmental model and by incidence data. Ref: Jorge, DCP et al. (2022). R. Soc. Open Sci. 9, 220005.

## [03871] Modelling human behavioural change during the outbreak of emerging infectious disease

**Format :** Talk at Waseda University

**Author(s) :** Ryosuke Omori (Hokkaido University)

**Abstract :** Disease dynamics like SARS-CoV-2 is difficult to describe by mathematical modelling. One of reasons is lack of knowledge of behavioral change due to the difficulty of measuring individual decision. To solve this problem, we defined index for the mobility avoidance in response to epidemic measured using accommodation reservation data and decision timing for behavioral change can be quantified. Using this index, we revealed general patterns in host behavioral change dynamics in response to SARS-CoV-2 outbreaks.

00309 (2/4) : 1D @A601 [Chair: Claudia P. Ferreira]

## [01440] Mathematical insights of chemical and Wolbachia-based mosquito control

**Format :** Talk at Waseda University

**Author(s) :** OLGA VASILIEVA (Universidad del Valle) Daiver Cardona-Salgado (Universidad Autonoma de Occidente) Lilian Sofia Sepulveda-Salcedo (Universidad Autonoma de Occidente)

**Abstract :** Wolbachia is a symbiotic bacterium that can block virus replication in Aedes aegypti mosquitoes, the primary transmitters of different vector-borne diseases. This thwarts the virus transmission from mosquitoes to humans. In recent years, Wolbachia-based biocontrol of Ae. aegypti mosquitoes have been gradually replacing the traditional control interventions based on insecticide spraying. In this presentation, we assess the pros and cons of Wolbachia-based biocontrol through the mathematical modeling of the mosquito population dynamics.

## [02743] ON THE ORIGIN OF COMPLEX DYNAMICS IN MULTI-STRAIN DENGUE MODELS

**Format :** Talk at Waseda University

**Author(s) :** Maira Aguiar (Basque Center for Applied Mathematics)

**Abstract :** Dengue fever epidemiological dynamics shows large fluctuations in disease incidence. Multi-strain models show complex dynamics and qualitatively a very good result when comparing empirical data and model simulations, however, the extent of biological mechanisms generating complex behavior in simple epidemiological models is still unexplored. In this talk, I will present a set of models motivated by dengue fever epidemiology and compare different dynamical behaviors originated when increasing complexity into the model framework.

## [04155] Covid-19: Vaccination impact after lockdown lifting and its large fluctuations

**Format :** Talk at Waseda University

**Author(s) :** Nico Stollenwerk (BCAM, Bilbao, Pais Vasco)

**Abstract :** The initial phase of the COVID-19 pandemic in beginning 2020 with exponential growth of infected and hospitalizations led to severe lockdown measures in many countries.

The subsequent lifting of the lockdowns prohibited new exponential growth, but lead to large subcritical fluctuations, with power law characteristics close to endemic thresholds, analysed for Basque Country data on a daily base for actual management purposes. We extended the modelling framework successfully into the vaccine introduction period.

## [03501] Optimization of Vaccination strategies on a metropolitan area

**Format :** Talk at Waseda University

**Author(s) :** Lucas Machado Moschen (School of Applied Mathematics - FGV EMAp) Maria Soledad Aronna (School of Applied Mathematics - FGV EMAp)

**Abstract :** We propose a model for vaccination in a network that models a typical metropolitan area. By employing tools of mathematical epidemiology and optimal control, we analyze the effectiveness of different allocation policies for distribution of vaccines and we search for optimal strategies.

00309 (3/4) : 1E @A601 [Chair: NONE - no section; talk 04326 is the same as 04328]

## [04326] Population Dynamics in Biology and Medicine

**Format :** Talk at Waseda University

**Author(s) :** Sunmi Lee (Kyung Hee University )

**Abstract :** The rapid spread of COVID-19 worldwide has highlighted the importance of non-pharmaceutical interventions. Policies that limit gatherings and enforce social distancing help to mitigate the spread of the disease, but also negatively impact the economy. Consequently, policymakers face the dilemma of whether to slow the outbreak by imposing strict rules or reduce the economic burden. This paper presents a novel framework for designing intervention policies based on deep reinforcement learning. The social distancing policies used by the South Korean government and their effects on the national economy are surveyed and integrated into a newly designed multi-patch epidemic model. The mobility between each pair of 17 patches (South Korean regions) is reconstructed using official data. The proximity policy optimization algorithm is adopted to optimize the policy model. The reward function incorporates the outbreak and economic loss, with an additional control variable that helps policymakers to determine the desired equilibrium between disease outbreak and economic recession. Our results highlight region-specific social distancing interventions compromising the dilemma between epidemic costs and economic costs.

00309 (4/4) : 2C @A601 [Chair: Maria Soledad Aronna]

## [04328] Population Dynamics in Biology and Medicine

**Format :** Talk at Waseda University

**Author(s) :** Sunmi Lee (Kyung Hee University ) Hyo Sun Lee (Kyung Hee University )

**Abstract :** The rapid spread of COVID-19 worldwide has highlighted the importance of non-pharmaceutical interventions. Policies that limit gatherings and enforce social distancing help to mitigate the spread of the disease, but also negatively impact the economy. Consequently, policymakers face the dilemma of whether to slow the outbreak by imposing strict rules or reduce the economic burden. This paper presents a novel framework for designing intervention policies based on deep reinforcement learning.

## [01337] A mathematical model to melanoma growth with macrophages and immunotherapy

**Format :** Talk at Waseda University

**Author(s) :** Paulo F. A. Mancera (UNESP) Jairo G Silva (IFMT) Mostafa Adimy (Inria and UCBL 1, Lyon France) Guilherme Rodrigues (UNESP)

**Abstract :** We present a new mathematical model based on ODE to describe the dynamics of melanoma under an immunotherapeutic treatment. The novelty of the proposed model is the inclusion of the tumor-associated macrophage (TAM) population, enabling the in silico analysis of its influence on the failure of this immunotherapy.

## [02941] A Mathematical Perspective on Resilience and Sustainability in Climate and Biodiversity

**Format :** Talk at Waseda University

**Author(s) :** Michel DE LARA (CERMICS - Ecole des Ponts ParisTech)

**Abstract :** In this talk, I will

- scan through the IPCC (climate) and IPBES (biodiversity) international bodies reports,
- address theoretical aspects: how can we formalize sustainability and resilience with tools from control theory (including viability) and decision under uncertainty?
- present methods: how can we tackle problem solving, once mathematically formalized?
- outline examples: biodiversity (fisheries, epidemiology), energy and climate,
- raise open questions and challenges, especially for the stochastic optimization community.

## [01827] Potential Impacts of Mass Nutritional Supplementation on Measles Dynamics

**Format :** Online Talk on Zoom

**Author(s) :** Navideh Noori (Institute for Disease Modeling, Bill & Melinda Gates Foundation) Laura A Skrip (School of Public Health, University of Liberia) Assaf P Oron (Institute for Health Metrics and Evaluation, University of Washington) Kevin A McCarthy (Institute for Disease Modeling, Bill & Melinda Gates Foundation) Joshua L Proctor (Institute for Disease Modeling, Bill & Melinda Gates Foundation) Guillaume Chabot-Couture (Institute for Disease Modeling, Bill & Melinda Gates Foundation) Benjamin M Althouse (Information School, University of Washington) Kevin P.Q. Phelan (The Alliance for International Medical Action (ALIMA)) Indi Trehan (Department of Pediatrics, Global Health, and Epidemiology, University of Washington)

**Abstract :** The bidirectional interaction between undernutrition and infection can be devastating to child health. Treatment of acute malnutrition can reverse some of its deleterious effects and reduce susceptibility to infection. To understand how integrating nutrition interventions and vaccination affects a vaccine-preventable disease dynamics, we developed a measles transmission model. We show leveraging mass nutritional supplementation as a contact point with the health system to increase measles vaccination coverage has a synergistic benefit beyond either intervention alone.

## [00316] Dynamics of patterns and traveling waves arising from reaction-diffusion systems

**Session Time & Room :**

00316 (1/2) : 5B (Aug.25, 10:40-12:20) @G501

00316 (2/2) : 5C (Aug.25, 13:20-15:00) @G501

**Type :** Proposal of Minisymposium

**Abstract :** Reaction-diffusion systems reveal rich phenomena related to mathematical biology and evolutionary dynamics, like pattern formation, propagation of traveling waves. These results are also related to the free boundary problems coming from the fast reaction limits. In order for the communication with other researchers, we organize a minisymposium consisting of the topics on patterns, traveling waves and entire solutions for reaction-diffusion systems. The speakers introduce their works from the approach by center manifold reduction, comparison principles and variational methods. We expect to have new and positive contributions to these fields.

**Organizer(s) :** Chueh-Hsin Chang, Chih-Chiang Huang

**Classification :** 35C07, 35K57, 35A15, 35R35, 35B08

**Minisymposium Program :**

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00316 (1/2) : 5B @G501 [Chair: Chang-Hong Wu]

## [03601] Cross-diffusion derived from predator-prey models with two behavioral states in predators

**Format :** Talk at Waseda University

**Author(s) :** Hirofumi Izuhara (University of Miyazaki)Masato Iida (University of Miyazaki)Ryusuke Kon (University of Miyazaki)

**Abstract :** Cross-diffusion may be an important driving force of pattern formation in population models. Recently, a relation between cross-diffusion and reaction-diffusion systems has been revealed from the mathematical modeling point of view. In this talk, we derive a predator-prey model with cross-diffusion from a simple reaction-diffusion system with two behavioral states in the predator population and examine whether cross-diffusion can induce spatial patterns in predator-prey models.

## [00453] Weak entire solutions of reaction-interface systems

**Format :** Talk at Waseda University

**Author(s) :** YANYU CHEN (National Taiwan University)

**Abstract :** In this talk, the singular limit problems arising from FitzHugh–Nagumo-type reaction–diffusion systems are studied, which are called reaction–interface systems. All weak entire solutions originating from finitely many excited intervals are completely characterized. For weak entire solutions originating from infinitely many excited intervals, periodic wave trains and time periodic solutions are discussed.

## [03042] Pulse bifurcations in a three-component FitzHugh-Nagumo system

**Format :** Talk at Waseda University

**Author(s) :** Kei Nishi (Kyoto Sangyo University)

**Abstract :** Pulse dynamics in a three-component FitzHugh-Nagumo system in one dimensional space is considered. The system admits a pulse solution of bistable type, which exhibits a variety of interface dynamics, not observed for the two-component FitzHugh-Nagumo system. In order to analytically investigate the mechanism for the pulse behavior, we apply the multiple scales method to the original reaction-diffusion system, and derive finite-dimensional ordinary differential equations which describe the motions of the pulse interfaces. The reduced ODEs enable us to reveal the global bifurcation structures of the pulse solutions, and to clarify the mechanism behind the variety of the pulse dynamics from a view point of bifurcation theory.

## [05009] The Motion of Weakly Interacting Waves for Reaction-Diffusion Equations in a Cylinder

**Format :** Talk at Waseda University

**Author(s) :** Chih-Chiang Huang (National Chung Cheng University )Shin-Ichiro Ei (Hokkaido University)

**Abstract :** In the talk, I am going to introduce the well-known results of the weakly interaction of two waves in a real line, for the Allen-Cahn equation, the FitzHugh-Nagumo system and competition-diffusion systems. Next, I would like to discuss such an interaction for reaction-diffusion equations with a triple-well potential in a cylinder. In this case, we can construct a stable traveling wave which is made up by two repulsive fronts. Based on a perturbation theory, the wave profile and wave speed can be characterized by a small parameter. This work is joint with Prof. Shin-Ichiro Ei.

00316 (2/2) : 5C @G501 [Chair: Hirofumi Izuhara]

## [02140] Some Progress on the spreading properties of two-species Lotka-Volterra competition-diffusion systems

**Format :** Talk at Waseda University

**Author(s) :** Chang-Hong Wu (National Yang Ming Chiao Tung University)

**Abstract :** The Lotka-Volterra competition-diffusion system is a well-established model for understanding the interactions between competing species. In particular, the two-species case has been extensively studied, revealing the existence of traveling waves that can provide insight into the spreading behaviors of the species. In this presentation, we will present some recent progress on the spreading properties of this system.

## [02366] Weak interaction between traveling wave solutions in the three-species competition-diffusion systems

**Format :** Talk at Waseda University

**Author(s) :** Chueh-Hsin Chang (National Chung Cheng University, Department of Mathematics)

**Abstract :** In this talk we consider the weak interaction between two trivial three-species traveling wave solutions (one component is trivial) of the threes-species Lotka-Volterra competition-diffusion systems. By the asymptotic behavior of the trivial threes-species waves and the existence results of the three-species waves from gluing bifurcation approaches in our previous results, we can observe the dynamics of the distance between the trivial three-species waves. The interaction between the two trivial three-species waves are attractive or repulsive due to different conditions of parameters. We let the growth rate of the third species as the bifurcation parameter.

## [04983] Defects in the segmented pattern for oscillated reaction-diffusion systems

**Format :** Talk at Waseda University

**Author(s) :** Ayuki Sekisaka (Meiji university)

**Abstract :** In this talk, the existence and stability of the modulated waves of a certain three-component reaction-diffusion system will be discussed. The modulated waves appearing in this equation are called defects, and their formulation and basic properties have been investigated by Sandstede and Scheel. In this talk, we will discuss the basic properties of the defects appearing in the equations and their stability using the infinite dimensional Evans function.

## [04560] Linearized eigenvalue problems in a mass-conserved reaction-diffusion compartment model

**Format :** Talk at Waseda University

**Author(s) :** Tsubasa Sukekawa (Institute for the Advanced Study of Human Biology (ASHBi), Kyoto University Institute for Advanced Study, Kyoto University)

**Abstract :** In a mass-conserved reaction-diffusion system, we can observe by numerical simulations that a transient pattern

such as a stripe one converges to a spatially monotone pattern.

To understand the dynamics theoretically, we introduce a reaction-diffusion compartment model. This model equation is defined on multiple regions (compartments), and each compartment is connected by diffusive coupling.

In this talk, we analyze linearized eigenvalue problems of spatially non-monotone stationary solutions in mass-conserved reaction-diffusion compartment model.

# [00319] Robust formulations for coupled multiphysics problems – Theory and applications

**Session Time & Room :**

00319 (1/5) : 1C (Aug.21, 13:20-15:00) @E710

00319 (2/5) : 1D (Aug.21, 15:30-17:10) @E710

00319 (3/5) : 1E (Aug.21, 17:40-19:20) @E710

00319 (4/5) : 2C (Aug.22, 13:20-15:00) @E710

00319 (5/5) : 2D (Aug.22, 15:30-17:10) @E710

**Type :** Proposal of Minisymposium

**Abstract :** The proposed minisymposium aims to bring together experts in the construction and analysis of novel discretization techniques for multiphysics models that maintain robustness with respect to model constants of interest. Particular emphasis will be placed on rigorous analysis of stability using saddle-point and perturbed saddle-point theory, a priori and a posteriori error estimation, as well on the design of robust solvers based on tailored domain decomposition techniques or on operator preconditioning. The session will also focus on the application of these new methodologies in the solution of coupled models arising in mechanobiology and similar multiphysics systems. For instance, our minisymposium features submissions involving brain tissue dynamics, cardiac electromechanics, and respiratory system

modeling; but it also welcomes talks related to geophysical flows or other types of fluid-structure interaction multiphysics problems.

**Organizer(s)** : Wietse Boon, Martin Hornkjøl, Miroslav Kuchta, Ricardo Ruiz Baier

**Classification** : 65N30, 65M30, 65F08

**Minisymposium Program :**

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00319 (1/5) : 1C @E710 [Chair: Ricardo Ruiz Baier]

## [01558] A diffuse interface method for fluid-poroelastic structure interaction

**Format** : Talk at Waseda University

**Author(s)** : Martina Bukač (University of Notre Dame)Boris Muha (University of Zagreb)Sunčica Čanić (University of California, Berkeley)

**Abstract** : The interaction between a free flowing fluid and a poroelastic structure, commonly formulated as a Navier-Stokes/Biot coupled system, has been used to describe problems arising in many applications, including environmental sciences, hydrology, geomechanics and biomedical engineering. Many existing numerical for this problem are based on a sharp interface approach, in the sense that the interface between the two regions is parametrized using an exact specification of its geometry and location, and the nodes in the computational mesh align with the interface. However, the exact location is sometimes not known, or the geometry is complicated, making a proper approximation of the integrals error-prone and difficult to automate. Hence, in this talk, we present a diffuse interface method for the coupled fluid-poroelastic structure interaction. The method uses a phase-field function which transitions from 1 in one region to 0 in the other region. We will first present the analysis of convergence of the discrete diffuse interface solution to the continuous sharp interface solution for the Stokes-Darcy problem. Then, we will discuss the extensions to Navier-Stokes/Biot system, and apply the method to study the optimal design of a bioartificial pancreas.

## [01781] Parameter-robust methods for the Biot-Stokes interfacial coupling

**Format** : Talk at Waseda University

**Author(s)** : Martin Hornkjøl (University of Oslo)Wietse Boon (KTH Royal Institute of Technology)Miroslav Kuchta (Simula Research Laboratory)Kent-Andre Mardal (University of Oslo)Ricardo Ruiz Baier (Monash University)

**Abstract** : In this talk I will discuss a fluid-structure interaction model of the monolithic coupling between the free flow of a viscous Newtonian fluid and a deformable porous medium separated by an interface. I will present a five-field mixed-primal finite element scheme, with a preconditioner, for solving the Stokes velocity-pressure and Biot displacement-total pressure-fluid pressure. With adequate inf-sup conditions the stability of the formulation is established robustly in all material parameters.

## [02817] Robust parallel solvers in cardiac modeling

**Format** : Talk at Waseda University

**Author(s)** : Nicolás Alejandro Barnafi Wittwer (University of Chile)

**Abstract** : We will see the physics involved in cardiac modeling, and focus on their efficient solution in an HPC infrastructure measured in both CPU time and scalability. As we will see, one of the main tools for improving performance is quasi-Newton methods, which do not sacrifice on scalability when initialized adequately. In some contexts, it will be possible to circumvent the solution of a linear system, which drastically reduces the complexity of the proposed solvers.

## [02934] Stochastic Galerkin mixed finite element approximation for poroelasticity with uncertain inputs

**Format** : Talk at Waseda University

**Author(s)** : Arbaz Khan (IIT Roorkee)Catherine E Powell (University of Manchester, UK)

**Abstract** : Linear poroelasticity models have important applications in biology and geophysics. In particular, the well-known Biot consolidation model describes the coupled interaction between the linear response of a porous elastic medium {saturated with fluid} and a diffusive fluid flow within it, assuming small deformations. This is the starting point for modeling human organs in computational medicine and for modeling the mechanics of permeable rock in geophysics. Finite element methods for Biot's consolidation model have been widely studied over the past four decades. In the first part of talk, we discuss a novel locking-free stochastic Galerkin mixed finite element method for the Biot consolidation model with uncertain Young's modulus and hydraulic conductivity field. After introducing a five-field mixed variational formulation of the standard Biot consolidation model, we discuss stochastic Galerkin mixed finite element approximation, focusing on the issue of well-posedness and efficient linear algebra for the discretized system. We introduce a new preconditioner for use with MINRES and establish eigenvalue bounds. Finally, we present specific numerical examples to illustrate the efficiency of our numerical solution approach. In the second part of the talk, we discuss a posteriori error estimators for SGFEM of Biot's consolidation model with uncertain inputs.

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00319 (2/5) : 1D @E710 [Chair: Rekha Khot]

## [03195] Finite element analysis for semilinear problems in liquid crystals

**Format :** Talk at Waseda University

**Author(s) :** Neela Nataraj (Professor )Ruma Maity (Postdoc Fellow)Apala Majumdar (Strathclyde University)

**Abstract :** A unified framework for the error control of different lowest-order finite element methods for approximating the regular solutions of systems of partial differential equations is established under a set of hypotheses.

The systems involve cubic nonlinearities in lower order terms, non-homogeneous Dirichlet boundary conditions, and the results are established under minimal regularity assumptions on the exact solution. The results for existence and local uniqueness of the discrete solutions using Newton-Kantorovich theorem and error control are presented.

The results are applied to conforming, Nitsche, discontinuous Galerkin, and weakly over penalized symmetric interior penalty schemes for variational models of ferromnematics liquid crystals.

## [01845] Twofold Saddle-Point Formulation of Biot Poroelasticity with Stress-Dependent Diffusion

**Format :** Talk at Waseda University

**Author(s) :** Ricardo Ruiz Baier (Monash University)Martin Hornkjøl (University of Oslo)Alberto Martin (Australian National University)Santiago Badia (Monash University)Kent-Andre Mardal (University of Oslo)Arbaz Khan (IIT Roorkee)

**Abstract :** We present a new stress/total-pressure formulation for poroelasticity that incorporates the coupling with steady nonlinear diffusion modified by stress. This nonlinear problem is written in mixed-primal form, which combines a perturbed twofold saddle-point system with an elliptic problem. We analyze the continuous formulation within the framework of abstract fixed-point theory and Fredholm alternative for compact operators. A mixed finite element method is proposed, and its stability and convergence are analyzed. The resulting model can be used to study the steady case of waste removal in the brain, providing insight into the transport of solutes in poroelastic structures under the influence of stress.

## [03220] Finite element analysis for the Navier-Lamé eigenvalue problem

**Format :** Talk at Waseda University

**Author(s) :** Jesus Vellojin (Universidad del Bío-Bío)Felipe Lepe (Universidad del Bío Bío)Gonzalo Rivera (Universidad de Los Lagos)

**Abstract :** In this talk, the author presents the eigenvalue problem for the Navier-Lamé system. The analysis of the spectral problem is based in the compact operators theory. A finite element method based in polynomials of degree  $k \geq 1$  is considered. An a posteriori error analysis is performed, where the reliability and efficiency of the proposed estimator is proved. A series of numerical tests are reported in order to assess the performance of the proposed numerical method.

## [04279] Isogeometric solvers for derived cardiac stem cell reaction-diffusion models

**Format :** Talk at Waseda University

**Author(s) :** Sofia Botti (Università della Svizzera Italiana and University of Pavia)Michele Torre (University of Pavia)

**Abstract :** Regenerative cardiology is recently employing human induced pluripotent stem cells derived cardiomyocytes to advance in patient-specific medicine. A multiphysics approach to the problem allows to couple the cardiac Monodomain reaction diffusion model with stem cell ionic models to simulate the action potential propagation in the engineered ventricle. The coupled model is then discretized using Isogeometric Analysis in space and finite differences in time to obtain a virtual representation of a derived cardiomyocytes ventricle.

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00319 (3/5) : 1E @E710 [Chair: Wietse Boon]

## [03598] Virtual element methods for Biot--Kirchhoff poroelasticity

**Format :** Talk at Waseda University

**Author(s) :** Rekha Mallappa Khot (Monash University)David Mora (Universidad del B'io-B'io)Ricardo Ruiz Baier (Monash University)

**Abstract :** We propose and analyse conforming and nonconforming virtual element formulations for the coupling of solid and fluid phases in deformable porous plates. The governing equations consist of one fourth-order equation for the transverse displacement of the middle surface coupled with a second-order equation for the pressure head relative to the solid. The discretisation supports arbitrary polynomial degrees on general polygonal meshes and we design companion

part\_1

operators with orthogonal properties and best-approximation estimate. We derive both a priori and a posteriori error estimates in appropriate norms, and these error bounds are robust with respect to the main model parameters. A few computational examples illustrate the properties of the numerical methods.

## [04832] Analyzing Multi-Dimensional Time-Dependent Solute Transport Models

**Format :** Talk at Waseda University

**Author(s) :** Marius Zeinhofer (Simula Research Laboratory)Rami Masri (Simula Research Laboratory)Miroslav Kuchta (Simula Research Laboratory)Marie Elisabeth Rognes (Simula Research Laboratory)

**Abstract :** We derive and analyze 3D-1D time dependent solute transport models for convection, diffusion, and exchange in and around pulsating vascular and perivascular networks from their 3D-3D counterpart. These models are applicable e.g.

for transport in vascularized tissue and brain perivascular spaces. We discuss existence and uniqueness questions, quantify the modelling error, discuss finite element discretizations and present numerical results. Technical key challenges are controlling constants in classical numerical analysis tools, such as Poincaré's inequality.

## [03951] Unfitted finite element methods for PDEs with dynamic interfaces and boundaries

**Format :** Talk at Waseda University

**Author(s) :** Santiago Badia (Monash University)Hridya Dilip (Monash University)Francesc Verdugo (Vrije Universiteit Amsterdam)Pere Antoni Martorell (Universitat Politècnica de Catalunya)

**Abstract :** In this presentation, we will present recent advances in the numerical approximation of PDEs with moving interfaces/boundaries using unfitted finite element methods. We will describe the numerical discretisation of transient problems using unfitted finite elements that are robust with respect to the small cut cell problems. We will design these algorithms for transient problems, e.g., by defining space-time discrete extension operators.

We will propose two different ways to design space-time unfitted methods. One approach is a pure space-time formulation, in which our geometries are considered in 4D (for a 3D problem in space). This approach is suitable, e.g., for problems in which the geometry is described via level sets. For complex geometrical representations in terms of oriented surface meshes, we propose a geometrical discretisation framework (for 3D in space) that provides all the quadrature rules needed to integrate our numerical methods on unfitted meshes. The extension of this 3D algorithm to 4D is a challenge.

We propose another space-time approach that solves the problem in the time-varying domain by using an extrusion of the 3D problem and a geometrical map. This way, one does not require 4D geometrical algorithms. In time, we consider discontinuous Galerkin spaces. The integration of inter-slab jump terms involves two functions on each side of the interface that are defined on different meshes (the background mesh and the mapped background mesh). In order to exactly compute these integrals, we propose to use intersection algorithms.

## [05346] A two-way coupled Stokes-Biot-transport model

**Format :** Talk at Waseda University

**Author(s) :** Sergio Caucao (Católica University Concepcion)Xing Wang (University of Pittsburgh)Ivan Yotov (University of Pittsburgh)

**Abstract :** We study mathematical and computational modeling for coupled fluid-poroelastic structure interaction with transport. The model is two-way coupled and nonlinear, with the velocity driving the transport and the concentration affecting the fluid viscosity. We use a Galerkin method, energy estimates, compactness arguments, and fixed point theory to establish well-posedness of the model. We study the finite element approximation of the model and obtain solvability, stability, and error estimates. Computational experiments are conducted to illustrate the theoretical convergence rates and the performance of the method for modeling physical flow and transport phenomena.

00319 (4/5) : 2C @E710 [Chair: Martin Hornkjøl ]

## [04578] Conservative and robust methods for the Biot-Brinkman equations in vorticity form

**Format :** Talk at Waseda University

**Author(s) :** Alberto Francisco Martin Huertas (Australian National University)Ruben Caraballo-Díaz (Universidad del Bío-Bío)Chansophea Wathanak In (Monash University)Ricardo Ruiz-Baier (Monash University)

**Abstract :** In this talk we present a new formulation, a suitable finite element method, along with robust/mesh-independent preconditioners, for the steady coupling of viscous flow in deformable porous media using divergence-conforming filtration fluxes. Apart from the well-posedness of the different formulations, and optimal error estimates,

our mathematical analysis confirms robustness of the different methods presented in the case of large Lamé parameters and small permeability and storativity coefficients. A few representative numerical examples are presented to back up the analysis.

## [04697] A five-field mixed formulation for stationary magnetohydrodynamic flows in porous media

**Format :** Talk at Waseda University

**Author(s) :** Jessika Camaño (Universidad Católica de la Santísima Concepción)

**Abstract :** We introduce a new mixed variational formulation for a stationary magnetohydrodynamic flows in porous media problem, whose governing equations are given by the steady Brinkman-Forchheimer equations coupled with the Maxwell equations. Unique solvability of the continuous and discrete systems has been proven.

Stability, convergence, and optimal a priori error estimates for the associated Galerkin scheme are obtained. Numerical tests illustrate the theoretical results.

## [04964] Domain decomposition solvers for problems with strong interface perturbations

**Format :** Online Talk on Zoom

**Author(s) :** Miroslav Kuchta (Simula Research Laboratory)

**Abstract :** Operators formed by an elliptic part in the bulk domain and a parameter weighted interface perturbation arise in

coupled multiphysics systems as solution operators or as part of their preconditioners. Such systems are often not amenable to off-the-shelf methods if robustness with respect to the coupling is to be retained. In this talk we develop robust and scalable solvers for interface-perturbed operators based on domain/subspace decomposition. We demonstrate performance of the algorithms for single and multiphysics problems such as the EMI and Darcy-Stokes equations.

## [04995] Numerical solution of the Biot/elasticity interface problem using virtual element methods

**Format :** Online Talk on Zoom

**Author(s) :** Nitesh Verma (Indian Institute of Technology Bombay)Ricardo Ruiz Baier (Monash University)David Mora (Universidad del Bío-Bío)Sarvesh Kumar (Indian Institute of Space Science and Technology)

**Abstract :** We propose, analyse and implement a virtual element discretisation for an interfacial poroelasticity/elasticity consolidation problem. The formulation of the time-dependent poroelasticity equations uses displacement, fluid pressure and total pressure, and the elasticity equations are written in the displacement-pressure formulation. The construction of the virtual element scheme does not require Lagrange multipliers to impose the transmission conditions (continuity of displacement and total traction, and no flux for the fluid) on the interface. We show the stability and convergence of the virtual element method for different polynomial degrees, and the error bounds are robust with respect to delicate model parameters (such as Lame constants, permeability, and storativity coefficient). Finally, we provide numerical examples that illustrate the properties of the scheme.

00319 (5/5) : 2D @E710 [Chair: Alberto F. Martin]

## [04946] A conforming finite element method for a nonisothermal fluid-membrane interaction

**Format :** Talk at Waseda University

**Author(s) :** Ricardo Oyarzúa (Universidad del Bío-Bío)

**Abstract :** We propose a conforming finite element method for a nonisothermal fluid-membrane interaction problem. The governing equations are given by a Navier-Stokes/Darcy system for the fluid variables and a convection-diffusion model for the temperature. Both systems are coupled through buoyancy terms and a set of transmission conditions on the fluid-membrane interface given by mass conservation, balance of normal forces, the Beavers-Joseph-Saffman law, and the continuity of the heat flux and the fluid temperature.

## [05072] Multipoint mixed finite elements for Biot poroelasticity using a rotation-based formulation

**Format :** Talk at Waseda University

**Author(s) :** Wietse Boon (Politecnico di Milano)Alessio Fumagalli (Politecnico di Milano)Anna Scotti (Politecnico di Milano)

**Abstract :** We propose a discretization method for Biot poroelasticity that employs the lowest-order Raviart-Thomas finite element space for the solid displacement and piecewise constants for the fluid pressure. The solid rotation and fluid flux are introduced as auxiliary variables and subsequently removed from the system using a local quadrature rule, leading to a multipoint rotation-flux mixed finite element method. By analyzing the method in terms of weighted norms, we additionally obtain parameter-robust preconditioners.

## [05593] Application of CutFEM to the modeling of coastal processes through vegetation

**Author(s) :** Chris Kees (Louisiana State University)Wen-Huai Tsao (Louisiana State University)

**Abstract :** We consider viscous and depth-averaged models of non-hydrostatic coastal wave propagation through vegetation. Our aim is to model wave height attenuation and momentum dissipation through marsh vegetation. Each model requires a significantly different set of numerical methods to achieve higher-order accuracy in a robust manner, and we will discuss several of these, including CutFEM and multiscale methods. Finally we present results on experimental data obtained from physical models of wave/structure interaction.

## [00322] Methodological advancement in rough paths and data science

**Session Time & Room :**

00322 (1/3) : 4C (Aug.24, 13:20-15:00) @E502

00322 (2/3) : 4D (Aug.24, 15:30-17:10) @E502

00322 (3/3) : 4E (Aug.24, 17:40-19:20) @E502

**Type :** Proposal of Minisymposium

**Abstract :** Rough path theory is an emerging mathematical technology that captures macroscopically interactions of highly oscillatory streamed data. Formally, it extends the domain of definition for the calculus of deterministic controlled differential equations, allowing them to be driven by complex signals, potentially rougher than Brownian motion. This area has built bidirectional connections with data science and machine learning, enabling the development of novel, mathematics-informed methods for efficiently analyzing time series data, e.g. PDE-based Signature kernel, path development layer with Lie group representation. This minisymposia series facilitates the discussion of new methodological innovations on this interface between rough paths and data science.

**Organizer(s) :** Hao Ni, Yue Wu

**Classification :** 60L20, 60L70, 60L10, 62M45

**Minisymposium Program :**

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00322 (1/3) : 4C @E502 [Chair: Harald Oberhauser]

## [01385] A real analytic view on signatures

**Format :** Talk at Waseda University

**Author(s) :** Josef Teichmann (ETH Zurich)Valentin Tissot-Daguette (Princeton U)

**Abstract :** We introduce classical (convenient) concepts of real analytic functions on path spaces and apply them to the approximation of path space functionals. We also provide an invariance theory perspective on the Hambly-Lyons theorem that signatures characterize paths up to tree like equivalences.

## [01366] PCF-GAN: generating sequential data via the characteristic function of measures on the path space

**Format :** Talk at Waseda University

**Author(s) :** Hao Ni (UCL)Hang Lou (UCL)Siran Li (Shanghai Jiao Tong University )

**Abstract :** Implicit Generative Models(IGMs) are powerful tools for generating high-fidelity synthetic data. However, they struggle to capture the temporal dependence of time-series data. To tackle this issue, we directly compare the path distributions via the characteristic function of measures on the path space(PCF) from rough path theory, which uniquely characterises the law of stochastic processes. We then develop a novel PCF-GAN model by incorporating PCF with IGM for time series generation, leading to significant performance boost.

## [01336] Nyström approximation and convex kernel quadrature

**Format :** Talk at Waseda University

**Author(s) :** Satoshi Hayakawa (University of Oxford)

**Abstract :** We will discuss a refined analysis of Nyström approximation for an integral operator based on statistical learning theory, and demonstrate how we can use these results to obtain an improved estimate of the performance of convex kernel quadrature rules that are given by the low-rank kernel of Nyström approximation.

## [01374] Taylor remainder estimate for rough differential equations

**Format :** Online Talk on Zoom

**Author(s) :** Danyu Yang (Chongqing University)

**Abstract :** We consider a remainder estimate for truncated Taylor expansion for differential equations driven by inhomogeneous geometric rough paths. The estimate can be applied to differential equations driven by general stochastic processes with a regular drift term. It can also be useful when dealing with differential equations driven by branched rough paths and quasi-geometric rough paths which are isomorphic to inhomogeneous geometric rough paths.

00322 (2/3) : 4D @E502 [Chair: Hao Ni]

## [01331] Optimal stopping with signatures

**Format :** Talk at Waseda University

**Author(s) :** Christian Bayer (Weierstrass Institute)John Schoenmakers (Weierstrass Institute)Paul Hager (Humboldt-Universität zu Berlin)Sebastian Riedel (University of Hagen)

**Abstract :** We propose a new method for solving optimal stopping problems under minimal assumptions on the underlying stochastic process  $X$ . We consider stopping times represented by functionals of the rough path signature  $\mathbb{X}^{<\infty}$ , and prove that maximizing over these classes of signature stopping times solves the original optimal stopping problem. Using the algebraic properties of the signature, we can then recast the problem as a deterministic optimization problem on the expected signature.

## [01439] Analysis on unparameterised path space: towards a coherent mathematical theory

**Format :** Talk at Waseda University

**Author(s) :** Thomas Cass (Imperial College London)William Turner (Imperial College London)

**Abstract :** The signature is a non-commutative exponential that appeared in the foundational work of K-T Chen in the 1950s. It is also a fundamental object in the theory of rough paths (Lyons, 1998). More recently, it has been proposed, and used, as part of a practical methodology to give a way of summarising multimodal, possibly irregularly sampled, time-ordered data in a way that is insensitive to its parameterisation. A key property underpinning this approach is the ability of linear functionals of the signature to approximate arbitrarily any compactly supported and continuous function on (unparameterised) path space. We present some new results on the properties of a selection of topologies on the space of unparameterised paths. We discuss various applications in this context. Based on joint work with Will Turner.

## [01370] On some stability results in mathematical finance via rough path theory

**Format :** Talk at Waseda University

**Author(s) :** CHONG LIU (ShanghaiTech University)

**Abstract :** In this talk I will present some recent progress on establishing some stability results in mathematical finance, e.g., in portfolio theory and utility maximization problems, via an approach of rough path theory.

## [01438] Kernels Methods for Stochastic Processes

**Format :** Talk at Waseda University

**Author(s) :** Harald Oberhauser (University of Oxford)

**Abstract :** Kernels provide a powerful approach to learning from structured data. An important case of structured data arises when there is a natural sequential order in a data point; classic examples are time series or text. I will talk about the signature kernel that allows the computation of inner products of the signature of paths after they've been lifted to paths evolving in an infinite-dimensional Hilbert space.

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00322 (3/3) : 4E @E502 [Chair: Yue Wu]

## [01994] Optimal approximation with path signatures

**Format :** Talk at Waseda University

**Author(s) :** Emilio Ferrucci (University of Oxford)

**Abstract :** Path signatures have been used extensively as a way of representing the information encoded in multimodal data streams. This choice of a feature set is motivated by the famous universality result of Hambly & Lyons, 2010 and the fact that a broad class of parametrisation-invariant functions of a stream can be arbitrarily well approximated as linear functions of its signature. However, not much is known on the quantitative aspects of such approximations, and, just like Taylor approximations of smooth functions, they can converge slowly. Moreover, just like monomials in a real variable, the signature may fail to be a basis, meaning a function on paths does not have a canonical coefficient corresponding to each coordinate iterated integral. In this talk we explore ways of addressing these issues.

## [01279] Using AI to Accelerate (S)PDE Solving

**Format :** Online Talk on Zoom

**Author(s) :** Qi Meng (Microsoft Research)

**Abstract :** Partial differential equations play an important role in science and engineering. Recently, AI emerged as a disruptive technique on scientific computing and could break the computational bottleneck on solving complex PDE systems via training deep neural network models. In this talk, I will introduce our recent work on AI accelerated PDE solving including DeepVortexNet and DLR-Net, which uses probabilistic representation and regularity features to achieve robust supervision signal and well-generalized neural network architecture, respectively.

## [00769] Markov Chain Cubature for Bayesian Inference

**Format :** Online Talk on Zoom

**Author(s) :** James Foster (University of Bath)

**Abstract :** Markov Chain Monte Carlo is widely regarded as the "go-to" approach for Bayesian inference and, due to the theory of stochastic differential equations, many physics-inspired MCMC algorithms can scale to high dimensions.

In this talk, we consider an alternative to Monte Carlo for SDE simulation known as "Cubature on Wiener Space". In particular, by applying SDE cubature and resampling particles in a spatially balanced manner, we introduce a novel interacting particle algorithm for Bayesian inference.

## [01377] Iterated integrals of Gaussian fields and ill-posedness of heat equations

**Author(s) :** Ilya Chevyrev (University of Edinburgh)

**Abstract :** In this talk, I will present a probabilistic method to show norm inflation, and thus local ill-posedness, for non-linear heat equations above scaling criticality. One of the motivations is a proof that the DeTurck-Yang-Mills heat flow is ill-posed on any Banach space that carries the 3D Gaussian free field, which complements recent well-posedness results. The method is inspired by work of Lyons, 1991, on iterated integrals of Brownian paths. Based on arXiv:2205.14350.

## [00323] Integrating rough paths into domain applications

**Session Time & Room :**

00323 (1/3) : 5B (Aug.25, 10:40-12:20) @E501

00323 (2/3) : 5C (Aug.25, 13:20-15:00) @E501

00323 (3/3) : 5D (Aug.25, 15:30-17:10) @E501

**Type :** Proposal of Minisymposium

**Abstract :** Streamed data are ubiquitous. In this context, a key challenge is to quantify our understanding and account for the interaction between channels. Rough path theory provides new insights for producing actionable inference for multimodal path-like data. The path signature is a mathematical object with desirable approximation properties and geometric interpretation which leads to more effective features and analysis. Further, the expected signature provides a powerful way to describe empirical measures on streams. Applications include award-winning machine learning methods in healthcare and finance, as well as commercial-quality Chinese handwriting software. We expose new challenges and work on applications in this area.

**Organizer(s) :** Terry Lyons, Lingyi Yang

**Classification :** 60L10, 60L90, 37M10, 68T07, 60L20, Applications of rough analysis, Signatures, Differential equation-inspired neural networks

**Minisymposium Program :**

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00323 (1/3) : 5B @E501 [Chair: Lingyi Yang]

## [01350] Signatures and Functional Expansions

**Format :** Online Talk on Zoom

**Author(s) :** Bruno Dupire (Bloomberg)Valentin Tissot-Daguette (Princeton University)

**Abstract :** Path dependent options can be generated by combinations of signatures. We focus on the case of one asset augmented with time. We construct an incremental basis of signature elements which allows us to write a smooth path dependent payoff as a converging series of signature elements. By recalling the main concepts of Functional Itô Calculus, a natural framework for path-dependence, we draw links between two approximation results, the Taylor expansion and the Wiener chaos decomposition. We also establish the pathwise Intrinsic Expansion and link it to Functional Taylor Expansion.

## [01349] Neural Stochastic PDEs: Resolution-Invariant Learning of Continuous Spatiotemporal Dynamics

**Format :** Talk at Waseda University

**Author(s) :** Maud Lemercier (University of Oxford)Cristopher Salvi (Imperial College London)Andris Gerasimovics (University of Bath )

**Abstract :** Neural SDEs are a class of physics-inspired neural networks that are particularly well-suited for modelling temporal dynamics. However, they may not be the most appropriate tool to model systems that vary both in space and in time. In this talk, I will present a way to address this issue, leveraging the notion of a mild solution of an SPDE. I will introduce the Neural SPDE model and demonstrate its ability to learn solution operators of PDEs with stochastic forcing from partially observed data.

## [01332] Neural Controlled Differential Equations: The Log-ODE Method

**Format :** Talk at Waseda University

**Author(s) :** Benjamin Walker (University of Oxford)

**Abstract :** Neural controlled differential equations (NCDEs) are a powerful approach to time-series modelling. Their output is a linear map of a CDE's solution, where the vector field is learnt and the control is a continuous interpolation of the input data. This work demonstrates that NCDEs can achieve start-of-the-art performance on long time-series given two modifications: ensuring the vector field is smooth by bounding its Lip(2)-norm, and applying the Log-ODE method to the learnt vector field.

## [01297] Nowcasting with signatures

**Format :** Talk at Waseda University

**Author(s) :** Lingyi Yang (Alan Turing Institute)Samuel Cohen (University of Oxford)

**Abstract :** Nowcasting refers to inference of the recent past, present, or near future. This is common in economics as key indicators, like GDP, are published with significant delays due to data collection/cleansing. The signature, a mathematical object arising from rough analysis, captures geometric properties and handles missing data from complex sampling patterns. We look at nowcasting with regression on signatures and show that this simple model subsumes the popular Kalman filter in theory and performs well in practice.

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00323 (2/3) : 5C @E501 [Chair: Lingyi Yang]

## [00458] Path-Dependent Neural Jump ODEs

**Format :** Talk at Waseda University

**Author(s) :** Florian Krach (ETH Zurich) Marc Nübel (ETH Zurich) Josef Teichmann (ETH Zurich)

**Abstract :** In this talk we discuss the problem of forecasting general stochastic processes using a path-dependent extension of the Neural Jump ODE (NJ-ODE) framework.

While NJ-ODE was the first framework to establish convergence guarantees for the prediction of irregularly observed time-series, these results were limited to data stemming from Itô-diffusions with complete observations, in particular Markov processes where all coordinates are observed simultaneously.

Here, we first revisit the NJ-ODE and its results and then generalise them to generic, possibly non-Markovian or discontinuous, stochastic processes with incomplete observations, by utilising the reconstruction properties of the signature transform.

These theoretical results are supported by empirical studies, where it is shown that the path-dependent NJ-ODE outperforms the original NJ-ODE framework in the case of non-Markovian data.

## [00499] Signature Methods for Outlier Detection

**Format :** Talk at Waseda University

**Author(s) :** Paola Arrubarrena (Imperial College London and DataSig) Terry Lyons (University of Oxford) Thomas Cass (Imperial College University) Maud Lemercier (University of Oxford and DataSig)

**Abstract :** An anomaly detection methodology is presented that identifies if a given observation is unusual by deviating from a corpus of non-contaminated observations. The signature transform is applied to the streamed data as a vectorization to obtain a faithful representation in a fixed-dimensional feature space. This talk is applied to radio astronomy data to identify very faint radio frequency interference (RFI) contaminating the rest of the data.

## [01312] Path Development Network with Finite-dimensional Lie Group

**Format :** Online Talk on Zoom

**Author(s) :** Hang Lou (University College London) Hao Ni (University College London) Siran Li (Shanghai Jiao Tong University)

**Abstract :** We propose a novel, trainable path development layer that exploits representations of sequential data through finite-dimensional Lie groups. The path development, which originates from rough path theory, inherits useful analytical properties from path signatures while also offering much richer group structures. Empirical results show the superiority of the development layer over signature features in terms of accuracy and dimensionality. The compact hybrid model, which stacks a one-layer LSTM with the development layer, achieves state-of-the-art performance against various RNN and continuous time series models on various datasets.

## [01355] From CCTV video streams to inferring NO<sub>2</sub> emissions at city-scale

**Format :** Online Talk on Zoom

**Author(s) :** Mohamed Ibrahim (University of Leeds) Terry Lyons (Oxford university)

**Abstract :** In this talk, we show how we can infer NO<sub>2</sub> emissions from CCTV video streams at city-scale through rough path theory. we introduce a framework for mapping objects in CCTV video streams as a stream of paths highlighting the order in which events take place. This temporal representation gives a descriptive summary for video contents which we can maximise: 1) data anonymity, and 2) systematic readability of large-scale video streams.

00323 (3/3) : 5D @E501 [Chair: Terry Lyons]

## [01359] Addressing bias adversarially in online learning.

**Format :** Online Talk on Zoom

**Author(s) :** Elena Gal (University of Oxford)

**Abstract :** We consider a class of online problems where the true label is only observed when a data point is assigned a positive label by a learner, eg for bank loans. In this setting the labelled training set suffers from accumulating bias since it is created by learners past decisions.

We propose to address the bias in the training set using adversarial domain adaptation. Our approach significantly exceeds SOTA on a set of challenging benchmark problems.

## [01353] Improving Training of Neural CDEs

**Format :** Online Talk on Zoom

**Author(s) :** Jason Michael Rader (University of Oxford)

**Abstract :** Neural CDEs are continuous-time analogues of recurrent neural networks which are effective at handling irregular time steps, densely sampled data, and long time series. We present recent advances in training neural CDEs in a

memory efficient manner for large-scale problems.

## [03470] From MMD-Regime detection to MMD-Generative Models with Applications

**Format :** Online Talk on Zoom

**Author(s) :** Blanka Horvath (University of Oxford)Zacharia Issa (King's College London)

**Abstract :** Time series data derived from asset returns are known to exhibit certain properties, termed stylised facts, that are consistently prevalent across asset classes and markets. For example, to name a few, asset price returns are widely accepted to be non-stationary, non-auto correlative, and to exhibit volatility clustering. We refer the reader to \cite{cont2001empirical} for a thorough discussion of such properties. In this article we will turn our attention to one property in particular, the heteroscedastic nature of financial time series, since it is of imminent practical relevance to financial analysts and quants for a multitude of practical applications. In this context, one may be interested in whether a given asset returns series---or a set of series, in case of multiple assets---can be divided into periods in which the (random) asset price dynamics can be attributed to the same underlying distribution (up to, perhaps, a small estimation error). Such periods are often referred to as market regimes, and we call the task of finding an effective way of grouping these regimes the market regime clustering problem (MRCP). This article is devoted to the online detection of such regimes, i.e. to developing tools that help us recognise in real time (as data comes in) if a shift in the underlying regime is happening.

## [01236] Capturing Graphs with Hypo-Elliptic Diffusions

**Format :** Online Talk on Zoom

**Author(s) :** Csaba Toth (University of Oxford)Derrick Lee (University of Oxford)Celia Hacker (MPI for Mathematics in the Sciences)Harald Oberhauser (University of Oxford)

**Abstract :** Convolutional layers within graph neural networks operate by aggregating information about local neighbourhood structures; one common way to encode such substructures is through random walks. The distribution of these random walks evolves according to a diffusion equation defined using the graph Laplacian. We extend this approach by leveraging classic mathematical results about hypo-elliptic diffusions. This results in a novel tensor-valued graph operator, which we call the hypo-elliptic graph Laplacian. We provide theoretical guarantees and efficient low-rank approximation algorithms.

## [00324] Minisymposium on Combinatorial Reconfiguration

**Session Time & Room :** 2E (Aug.22, 17:40-19:20) @G302

**Type :** Proposal of Minisymposium

**Abstract :** Combinatorial reconfiguration is an emerging branch of discrete mathematics that deals with gradual changes of combinatorial objects. While several related concepts have been studied over the years from different perspectives, the theory is growing up by combining its mathematical, computational and practical aspects.

This minisymposium aims at communicating recent research trends on combinatorial reconfiguration and discussing possible future directions.

**Organizer(s) :** Takehiro Ito, Yusuke Kobayashi, Yoshio Okamoto

**Classification :** 05Axx, 05Cxx, 52Cxx, 52Bxx

**Minisymposium Program :**

00324 (1/1) : 2E @G302 [Chair: Yoshio Okamoto]

## [04748] Invitation to Combinatorial Reconfiguration

**Format :** Talk at Waseda University

**Author(s) :** Takehiro Ito (Tohoku University)

**Abstract :** Combinatorial Reconfiguration studies reachability and related questions over combinatorial structures. A typical example asks if the solution space of a Boolean formula is connected with respect to the Boolean cube topology, formed by flipping one bit at the time. Reconfiguration problems have been studied intensively in this decade from the algorithmic viewpoints. In this talk, we will give a broad introduction of combinatorial reconfiguration, and show some recent progress on the topic.

## [04759] Geometric algorithms for reconfiguring modular robots

**Format :** Online Talk on Zoom

**Author(s) :** Irene Parada (BarcelonaTech (UPC))

**Abstract :** Modular self-reconfigurable robots consist of units that can move and connect to form larger shapes. A central problem is how to efficiently reconfigure between shapes while maintaining connectivity. We explore the computational complexity of this reconfiguration problem for the most fundamental lattice-based models of modular robots. Some lattices and moves allow for efficient reconfiguration algorithms, while in other models the problem is PSPACE-complete. For those cases, we identify simple conditions that guarantee universal reconfigurability.

## [05218] Toric Promotion and Permutoric Promotion

**Format :** Online Talk on Zoom

**Author(s) :** Colin Defant (Massachusetts Institute of Technology)

**Abstract :** We introduce toric promotion and, more generally, permutoric promotion operators. These operators, which are variants of Schützenberger's famous promotion operator, act on labelings of a graph. We highlight cases where these operators have surprisingly nice orbit structures. Our investigation of permutoric promotion is surprisingly involved and relies on the analysis of gliding globes, sliding stones, and colliding coins. This work on permutoric promotion is joint with Rachana Madhukara and Hugh Thomas.

## [04747] Triangulations of cyclic polytopes through the lens of reconfiguration

**Format :** Talk at Waseda University

**Author(s) :** Nicholas James Williams (Lancaster University)

**Abstract :** We discuss the reconfiguration problem given by taking the set of triangulations of a cyclic polytope as the state space, with the reconfiguration moves given by bistellar flips (the higher-dimensional analogue of flipping a diagonal within a quadrilateral). The state space is connected, and we will outline how this is proven using a certain partial order on the states called the higher Stasheff-Tamari order. We will further consider as many different other aspects of the reconfiguration as time permits, including the significance of triangulations of higher-dimensional cyclic polytopes for reconfigurations of lower-dimensional cyclic polytopes, efficient combinatorial descriptions of triangulations of cyclic polytopes, and the diameter of the state space.

# [00336] Recent advances in Optimization methods with applications

**Session Time & Room :** 1E (Aug.21, 17:40-19:20) @F312

**Type :** Proposal of Minisymposium

**Abstract :** The aim of this session is to present recent advances in optimization (e.g. calculus of variations, control theory, decision theory, etc). We are interested in its different approaches: theoretical, numerical analysis or applications to real life. Potential topics include, but are not limited to: Optimization, Numerical Mathematics, Optimal Control, Calculus of Variations, consensus theory, Mathematical Modeling, Dynamical Systems, Applications to Physics, Biology, Medicine and Robotics, and fractional calculus.

**Organizer(s) :** Ricardo Almeida, Natália Martins

**Classification :** 47N10, 65K10, 34B60, 26A33

**Minisymposium Program :**

00336 (1/1) : 1E @F312 [Chair: Ricardo Almeida]

## [02720] HABITAT LOSS AND COOPERATIVE HUNTING ON A THREE-SPECIES TROPHIC SYSTEM

**Format :** Talk at Waseda University

**Author(s) :** Jorge Duarte (Instituto Superior de Engenharia de Lisboa)Cristina Januário (Instituto Superior de Engenharia de Lisboa)Nuno Martins (Instituto Superior Técnico)

**Abstract :** Changes in ecosystems progress at a rapid pace mainly due to the climate crisis and human-induced perturbations. Researchers have used mathematical models to understand how species respond to these changes in habitat in order to ultimately forecast species extinctions and develop efficient conservation strategies. Our work highlights the fragility of predators hunting cooperatively under the loss of habitat.

## [02816] Modeling of impulsive perturbations by generalized fractional differential equations

**Format :** Talk at Waseda University

**Author(s) :** Snehana Hristova (Plovdiv University)

**Abstract :** The main aim is to emphasize on the statement of the impulsive perturbations in fractional differential equations. It will be considered two types of impulses- instantaneous impulses and non-instantaneous ones. To be more general we will consider the generalized proportional fractional derivatives of both Caputo type and Riemann-Liouville type in differential equations. Some existence results as well as stability properties of the solutions will be presented.

## [02710] Necessary conditions to optimize functionals involving a generalized fractional derivative

**Format :** Talk at Waseda University

**Author(s) :** Ricardo Almeida (University of Aveiro)

**Abstract :** In this work we combine two ideas: fractional derivatives of variable order and fractional derivatives depending on another function. With such operators, we develop a variational problem theory by presenting necessary conditions of optimization. The fundamental problem will be addressed, proving an Euler-Lagrange equation, and then other versions will be considered such as the isoperimetric problem or the Herglotz problem. An integration by parts formula is also proven. To end, we provide a numerical tool to solve fractional problems dealing with such fractional derivatives. The main idea is to approach the fractional derivative by an expansion formula in terms of integer order derivatives and then rewrite the fractional problema as a classical one.

## [02725] Herglotz's Variational Problem involving distributed-order fractional derivatives with arbitrary kernels

**Format :** Talk at Waseda University

**Author(s) :** Natália Martins (University of Aveiro)

**Abstract :** In this talk we extend the study of fractional variational problems of Herglotz type for the case where the Lagrangian function depends on distributed-order fractional derivatives with arbitrary smooth kernels, the endpoints conditions, and a real parameter. The fact that the Lagrangian depends on the boundary conditions and an arbitrary parameter is not an artificial generalization, as this formulation is important in many problems, such as in physics and economics.

## [00340] New trends in phase fields: theory & applications

**Session Time & Room :**

00340 (1/5) : 2D (Aug.22, 15:30-17:10) @E701

00340 (2/5) : 2E (Aug.22, 17:40-19:20) @E701

00340 (3/5) : 3C (Aug.23, 13:20-15:00) @E701

00340 (4/5) : 3D (Aug.23, 15:30-17:10) @E701

00340 (5/5) : 3E (Aug.23, 17:40-19:20) @E701

**Type :** Proposal of Minisymposium

**Abstract :** The phase field method is a powerful numerical method to solve moving boundary problems appearing in Materials Science and Engineering. Phase field theories are parameterized by a set of physically motivated variables and their governing equations. This mini-symposium will bring together numerical analysts and computational scientists working on phase field methods to present their recent advances in algorithm designs and applications of phase field methods. The main purposes of this mini-symposium are to review the current status, identify problems and future directions, and to promote phase field methods to a wider scientific and engineering community.

**Organizer(s) :** Mejdi Azaiez, Chuanju Xu

**Classification :** 65M06, 65M12, 65M70, 35R37

**Minisymposium Program :**

## [04343] Energy stability of variable step higher order ETD-MS scheme for gradient flows

**Author(s)** : Xiaoming Wang (Missouri University of Science and Technology)

**Abstract** : We present a family of ETD-MS based variable-step higher order numerical schemes for a family of gradient flows. We demonstrate the energy stability of this family of numerical algorithms. Numerical examples will be provided to show the effectiveness of the schemes.

## [04034] Energy Dissipation of Time-Fractional Phase-Field Equations: Analysis and Numerical methods

**Author(s)** : Jiang Yang (Southern University of Science and Technology)

**Abstract** : There exists a well defined energy dissipation law for classical phase-field equations, i.e., the energy is non-increasing with respect to time. However, it is not clear how to extend the energy definition to time-fractional phase-field equations so that the corresponding dissipation law is still satisfied. In this work, we will try to settle this problem for phase-field equations with Caputo time-fractional derivative, by defining a nonlocal energy as an averaging of the classical energy with a time-dependent weight function. To deal with this, we propose a new technique on judging the positive definiteness of a symmetric function, that is derived from a special Cholesky decomposition. Then, the nonlocal energy is proved to be dissipative under a simple restriction of the weight function. Within the same framework, the time fractional derivative of classical energy for time-fractional phase-field models can be proved to be always nonpositive. At the discrete level, a fast L2-1<sub>σ</sub> method on general nonuniform meshes is employed. The global-in-time  $H^1$ -stability is established via the same framework.

## [02973] A Spectral Element in Time Method for Nonlinear Gradient Systems

**Author(s)** : Shiqin Liu (University of Chinese Academy of Sciences)Haijun Yu (Academy of Mathematics and Systems Science, Chinese Academy of Sciences)

**Abstract** : We present a spectral element in time method for large scale nonlinear gradient systems, with the phase-field Allen-Cahn equation as an example. Different to commonly-used spectral in time methods that employ Petrov-Galerkin or weighted Galerkin approximations, the present method employs a natural variation Galerkin form that maintains volume conservation and energy dissipation property of the continuous dynamical systems. Explicit extrapolation is applied to handle the nonlinear term, which makes the method efficient. The explicit method can be improved by a few Picard iterations to obtain superconvergence. Numerical experiments confirm that the method outperforms the popular BDF4 scheme and the ETD-RK4 method.

## [02987] Energy stability and error analysis of high-precision algorithms for two-phase incompressible flows

**Author(s)** : Xiaoli Li (Shandong University)

**Abstract** : In this talk, we will first present several efficient and high-precision schemes for the two-phase incompressible flows. These schemes are linear, decoupled and only require solving a sequence of Poisson type equations at each time step. We carry out a rigorous error analysis for the first-order scheme, establishing optimal convergence rate for all relevant functions in different norms. Next we shall discuss the consistent splitting GSAV approach for the Navier-Stokes equations and carry out theoretical analysis.

00340 (2/5) : 2E @E701

## [03070] NONLOCAL CAHN-HILLIARD TYPE MODEL FOR IMAGE INPAINTING

**Author(s)** : Majdi AZAIEZ (Bordeaux INP & I2M UMR 5295)Dandan JIANG (Xiamen University)Chuanju Xu (Xiamen University)Alain Miranville (Poitier University)

**Abstract** : In this talk, we propose a Cahn-Hilliard type nonlocal model for image inpainting which is equipped with a nonlocal diffusion operator for image inpainting. For its approximation we use the modified convex splitting method for the temporal discretization with the non-local diffusion term treated implicitly, and the fidelity term treated explicitly. Spatial discretization is performed by the Fourier collocation method. We will provide several numerical experiments to assess the efficiency of our method.

## [03100] A Variety of Gradient Flows: Modeling and Numerical Methods

**Author(s)** : Chuanju Xu (Xiamen University)

**Abstract** : In this talk I will discuss a variety of gradient flow models for multi-phase problems, derived from an energy variational formulation. The models includes fractional differential equations, equations describing the interfacial dynamics of immiscible and incompressible two-phase fluids, dendritic crystal growth model, thermal phase change problems etc.

The talk starts with a review of the models and numerical methods for these models.

Then a new class of time-stepping schemes will be discussed.

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00340 (3/5) : 3C @E701

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00340 (4/5) : 3D @E701

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00340 (5/5) : 3E @E701

## [00341] Graph Coloring

**Session Time & Room** : 4E (Aug.24, 17:40-19:20) @A617

**Type** : Proposal of Minisymposium

**Abstract** : Graph coloring are fundamental objects of study in graph theory and have many applications including theoretical computer science, scheduling problems, and mobile phone network problems.

Beginning with the four color theorem, many conjectures and extensions of graph coloring have been proposed. In addition, relationships with other subjects of graph theory have also been discovered.

However, despite the efforts of many mathematicians, there are still many unsolved problems in graph coloring. In this mini-symposium, we will explore the latest topics and results concerning coloring conjectures, extensions, and relationships with other subjects.

**Organizer(s)** : Shunichi Maezawa

**Classification** : 05C15, 05C10

**Minisymposium Program** :

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00341 (1/1) : 4E @A617 [Chair: Shunichi Maezawa]

## [02669] Flows and coloring of triangle-free graphs on surfaces

**Format** : Talk at Waseda University

**Author(s)** : Zdeněk Dvořák (Charles University)

**Abstract** : The near-quadrangulations of surfaces, i.e., graphs where almost all faces have length four, play an important role in the theory of 3-colorability of triangle-free graphs on surfaces. We present a powerful approach to coloring near-quadrangulations using nowhere-zero flows and explore its applications. In particular, we show a connection between the maximum edgewidth of triangle-free non-3-colorable graphs on a given surface and a long-standing conjecture concerning the maximum width of polytopes containing no integer points.

## [02782] Alon-Tarsi number of planar graphs

**Format** : Online Talk on Zoom

**Author(s)** : Xuding Zhu (Zhejiang Normal University) Yangyan Gu (Zhejiang Normal University)

**Abstract** : This talk presents a simple proof of the result that planar graphs have Alon-Tarsi number at most 5, and that each planar graph  $G$  has a matching  $M$  such that  $G - M$  has Alon-Tarsi number at most 4. The former result is a strengthening of Thomassen's result that planar graphs are 5-choosable, and the latter result implies that every planar graph  $G$  has a matching  $M$  such that  $G - M$  is online 4-choosable, which is a generalization of Cushing-Kierstead's result that planar graphs are 1-defective 4-choosable.

## [02488] Edge-colourings, hamiltonian cycles, and a problem of Kotzig

**Format** : Online Talk on Zoom

**Author(s)** : Carol T. Zamfirescu (Ghent University)

**Abstract** : This talk concerns proper edge-colourings of regular graphs in which certain colour pairs form hamiltonian cycles -- such a pair is called perfect. We present a theorem solving Kotzig's problem asking whether planar 5-regular

graphs exist admitting an edge-colouring in which all ten pairs are perfect. If time permits, we shall also discuss certain edge-colouring enumeration problems. This talk is based on joint work with Nico Van Cleemput.

### [03108] Coloring Graphs with Forbidden Minors

**Format :** Online Talk on Zoom

**Author(s) :** Zi-Xia Song (University of Central Florida)Michael Lafferty (University of Central Florida)

**Abstract :** Hadwiger's Conjecture from 1943 states that every graph with no  $K_t$  minor is  $(t - 1)$ -colorable; it remains open for all  $t \geq 7$ . Jakobsen in 1971 proved that every graph with no  $K_7^{-2}$  minor is 6-colorable. In this talk, we present our recent work that every graph with no  $K_8^{-4}$  minor is 7-colorable, and every graph with no  $K_9^{-6}$  minor is 8-colorable, where  $K_t^{-s}$  denote the family of graphs obtained from  $K_t$  by removing  $s$  edges.

## [00342] Localized waves in nonlinear discrete systems

**Session Time & Room :**

00342 (1/2) : 4D (Aug.24, 15:30-17:10) @F308

00342 (2/2) : 4E (Aug.24, 17:40-19:20) @F308

**Type :** Proposal of Minisymposium

**Abstract :** There are various spatially discrete nonlinear media in nature and engineering systems as diverse as solid crystal, metamaterial, and optical waveguide array, etc. Such media are mathematically modeled by nonlinear lattice dynamical systems. In both of experimental and mathematical systems, nonlinear localized waves such as solitons and discrete breathers are widely observed. The nonlinear localized waves have attracted much interest from the point of view of applied mathematics and that of physics problems such as thermalization and charge transport. So, mathematical and/or numerical analyses have been actively made. This MS aims at sharing and discussing recent results on the topic.

**Organizer(s) :** Kazuyuki Yoshimura, Yusuke Doi

**Classification :** 37K60, 70K75, 70H12, 37M05, Nonlinear physics, Analysis and applications of waves in nonlinear discrete systems

**Minisymposium Program :**

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00342 (1/2) : 4D @F308 [Chair: Yusuke Doi]

### [00658] Existence of multi-pulse discrete breathers in Fermi-Pasta-Ulam-Tsingou lattices

**Format :** Talk at Waseda University

**Author(s) :** Kazuyuki Yoshimura (Tottori University)

**Abstract :** Discrete breathers are spatially localized periodic solutions in nonlinear lattices. We prove the existence of odd symmetric, even symmetric, and multi-pulse discrete breathers in strong localization regime in one-dimensional infinite Fermi-Pasta-Ulam-Tsingou (FPUT) lattices with even interaction potentials. The multi-pulse discrete breather consists of an arbitrary number of the odd-like and/or even-like primary discrete breathers located separately on the lattice. The proof applies to both cases of pure attractive and repulsive-attractive interaction potentials.

### [01557] Spectral properties of nonlinear excitations in semiclassical systems with charge transport

**Format :** Online Talk on Zoom

**Author(s) :** Juan FR Archilla (Universidad de Sevilla)Janis Bajars (University of Latvia)Yusuke Doi (Osaka University)Masayuki Kimura (Setsunan University)

**Abstract :** We study the spectral properties of polarobreathers, that is, breathers carrying charge in a semi-classical model. Lattice particles are described mathematically, while the charged particle is described as a quantum one within the tight-binding approximation. Three different spectra are considered: the spectra of the atom positions, the spectra of the charge carrier probability and the spectra of charge carrier probability amplitude. The observed spectrum properties are related with the physical properties of the semiclassical system.

**[01269] Nonlinear waves in multistable mechanical metamaterials****Format :** Talk at Waseda University**Author(s) :** Hiromi Yasuda (Japan Aerospace Exploration Agency) Hang Shu (University of Pennsylvania) Weijian Jiao (University of Pennsylvania) Vincent Tournat (Institut d'Acoustique - Graduate School (IA-GS), CNRS, Le Mans Université) Jordan R. Raney (University of Pennsylvania)**Abstract :** We explore collision behaviors of nonlinear waves in a multistable mechanical system with coupling between translational and rotational degrees of freedom. We show that the system can support two different types of nonlinear waves, specifically elastic vector solitons and topological solitons. Moreover, we experimentally and numerically demonstrate the nucleation of topological solitons via collisions of vector solitons. Our findings show a new potential way of generating and controlling nonlinear waves in a mechanical structure.**[01230] Soliton billiards****Format :** Online Talk on Zoom**Author(s) :** Jesus Cuevas-Maraver (University of Seville)**Abstract :** A point particle elastically reflected within an enclosed 2D domain is known as a billiard. Depending on the features of this domain, the trajectory of the particle can be closed or ergodic. In this talk, we show the similarities and differences when, instead of a classical particle, a soliton is scattered from closed 2D potentials. To this aim, we have considered a 2D NLS equation with saturable nonlinearity and square barriers (among other potentials).

00342 (2/2) : 4E @F308 [Chair: Kazuyuki Yoshimura]

**[00812] Universality Classes for Nonlinear Wave Thermalization****Format :** Talk at Waseda University**Author(s) :** Sergej Flach (Institute for Basic Science)**Abstract :** We study the slowing down of thermalization of many-body dynamical systems upon approaching integrable limits. We identify two fundamentally distinct long-range and short-range classes. The long-range class results in a single parameter scaling of the Lyapunov spectrum, with the rescaled spectrum approaching an analytical function. The short-range class results in a rescaled Lyapunov spectrum approaching a non-analytic function through an exponential suppression of all Lyapunov exponents relative to the largest one.**[01278] Numerical experiment on nonlinear localized oscillation propagating in a mass-spring chain****Format :** Talk at Waseda University**Author(s) :** Yosuke Watanabe (Setsunan University) Yusuke Doi (Osaka University)**Abstract :** Nonlinear localized oscillations excited and propagated in a mass-spring chain are studied. Letting the mass at one end of the chain driven sinusoidally at high frequency and large amplitude, localized oscillations can be excited intermittently near the end and propagated down the chain one after another at a constant speed. This phenomenon is known as supratransmission. We have experimentally observed the supratransmission by a mechanical mass-spring chain which emulates the Fermi-Pasta-Ulam one of beta type. The experimental results are compared with the numerical ones.**[01274] Moving Intrinsic Localized Modes Created by Transforming Wavenumber-frequency Spectrum of a Static Intrinsic Localized Mode in FPUT-NKG Mixed Lattices****Format :** Talk at Waseda University**Author(s) :** Masayuki Kimura (Setsunan University) Kosuke Kawasaki (Kyoto University) Shinji Doi (Kyoto University)**Abstract :** Intrinsic localized mode (ILM), also known as discrete breather (DB), is a spatially localized vibration in nonlinear lattices. It is well known that ILM can travel the lattices without decay of energy localization for a long period of time. In this study, initial values of moving ILMs with arbitrary speed are created by transforming the wavenumber-frequency spectrum of a static ILM. We will discuss the characteristics of the created moving ILMs.

## [00992] Structure of pairwise interaction symmetric lattice for moving discrete breather

**Format :** Talk at Waseda University

**Author(s) :** Yusuke Doi (Osaka University)Kazuyuki Yoshimura (Tottori University)

**Abstract :** The mobility of discrete breathers is an essential issue from the viewpoint of energy transport in microstructure and nanostructures. In this presentation, we construct a nonlinear lattice with long-range interaction, which supports the smooth mobility of the discrete breather by considering the invariance of the interaction potential to a certain mapping corresponding to the translational manipulation of the waveform. Numerical results on the dynamics of the discrete breather in the constructed lattice are also presented.

## [00345] Recent Developments for High-frequency Waves and Tomography

**Session Time & Room :**

00345 (1/2) : 3C (Aug.23, 13:20-15:00) @G808

00345 (2/2) : 3D (Aug.23, 15:30-17:10) @G808

**Type :** Proposal of Minisymposium

**Abstract :** Wave propagation is ubiquitous in our daily life, yet computing wave motion efficiently and accurately is still challenging in the high-frequency regime in many practical applications, such as nano-optics, material sciences, and geosciences. This mini-symposium gathers researchers in the field and provides a forum to exchange new ideas on recent theoretical and computational developments in high-frequency wave propagation and optics, as well as significant applications in medical and seismic tomography.

**Organizer(s) :** Jianliang Qian, Shingyu Leung

**Classification :** 35R30, 86A22, 35L05

**Minisymposium Program :**

00345 (1/2) : 3C @G808 [Chair: Jianliang Qian]

## [03696] Learning based on data and numerical solutions for differential equations

**Format :** Talk at Waseda University

**Author(s) :** Jin Cheng (Professor)Yu Chen (Dr.)

**Abstract :** Numerical methods for partial differential equations are the important and powerful tools for the engineering problems. The study of numerical methods for PDE is one of the hottest research topics in the applied mathematics and computational mathematics. Based on ideas from data learning, we propose a new method for finding numerical solutions of differential equations effectively, especially for the Helmholtz equations with the high wave numbers. The main idea of this method is to construct the approximation solutions by utilizing the relevant information from the solution we already have, which include the explicit solutions, the measured data from the experiments, the expression of the basic solution and the numerical solution obtained from the numerical experiments, etc. This is also a fast and high-precision numerical algorithm. It is shown that, especially for high-frequency problems, this method provides feasible solutions.

## [01633] Butterfly-compressed Hadamard-Babich Integrator for High-Frequency Helmholtz and Maxwell Equations in Inhomogeneous Media

**Format :** Talk at Waseda University

**Author(s) :** Yang Liu (Lawrence Berkeley National Laboratory)Jian Song (Michigan State University)Robert Burridge (University of New Mexico)Jianliang Qian (Michigan State University)

**Abstract :** We present a butterfly-compressed representation of the Hadamard-Babich (HB) ansatz for the Green's function of the high-frequency Helmholtz and Maxwell equations in smooth inhomogeneous media with arbitrary excitation sources. The proposed algorithm first solves the phase and HB coefficients via eikonal and transport equations using a coarse mesh, and then compresses the resulting HB interactions using several newly developed butterfly algorithms, leading to an optimal CPU complexity for any bounded 3D domains.

## [02074] Development and Analysis a higher-order numerical method for Helmholtz equation with high wave number

**Format :** Talk at Waseda University

**Author(s) :** Wenyuan Liao (University of Calgary)

**Abstract :** Numerical solution of the Helmholtz equation with high wave numbers is a challenging task due to several reasons, such as the large size and indefiniteness of the discrete linear system. In this talk, we introduce a new iterative method which is motivated by the idea of the normal equation method. We then solve the equivalent positive definite normal equation. Combined with acceleration techniques, the new method is efficient and accurate for solving the Helmholtz equation.

## [02172] Fixed Angle Inverse Scattering For Velocity

**Format :** Talk at Waseda University

**Author(s) :** Rakesh Rakesh (University of Delaware)

**Abstract :** An inhomogeneous acoustic medium is probed by a plane wave and the resultant time dependent wave is measured on the boundary of a ball enclosing the inhomogeneous part of the medium. We describe our partial results about the recovery of the velocity of the medium from the boundary measurement. This is a formally determined inverse problem for the wave equation, consisting of the recovery of a non-constant coefficient of the principal part of the operator from the boundary measurement.

00345 (2/2) : 3D @G808 [Chair: Shingyu Leung]

## [02057] Eulerian PDE methods for complex-valued eikonals in attenuating media

**Format :** Online Talk on Zoom

**Author(s) :** Jiangtao Hu (Chengdu University of Technology)Jianliang Qian (Michigan State University)Shingyu Leung (The Hong Kong University of Science and Technology)

**Abstract :** Seismic waves in earth media usually undergo attenuation. In the regime of high-frequency asymptotics, a complex-valued eikonal is essential for describing wave propagation in attenuating media. Conventionally, it is computed by ray-tracing methods defined by ODEs, but those irregularly distributed results hinder their applications. This talk proposes a unified eulerian PDE for several popular real ray-tracing methods. We also develop a highly accurate numerical scheme using factorization and LxF-WENO scheme.

## [01878] Uniformly convex neural networks and iterated network Tikhonov (iNETT) method

**Format :** Online Talk on Zoom

**Author(s) :** Davide Bianchi (Harbin Institute of Technology, Shenzhen)Guanghao Lai (Harbin Institute of Technology, Shenzhen)Wenbin Li (Harbin Institute of Technology, Shenzhen)

**Abstract :** We propose a non-stationary iterated network Tikhonov (iNETT) method for the solution of ill-posed inverse problems. The iNETT employs deep neural networks to build a data-driven regularizer, and it avoids the difficult task of estimating the optimal regularization parameter. To achieve the theoretical convergence of iNETT, we introduce uniformly convex neural networks to build the data-driven regularizer. Rigorous theories and detailed algorithms are proposed for the construction of convex and uniformly convex neural networks. In particular, given a general neural network architecture, we prescribe sufficient conditions to achieve a trained neural network which is component-wise convex or uniformly convex; moreover, we provide concrete examples of realizing convexity and uniform convexity in the modern U-net architecture. With the tools of convex and uniformly convex neural networks, the iNETT algorithm is developed and a rigorous convergence analysis is provided. Lastly, we show applications of the iNETT algorithm in 2D computerized tomography, where numerical examples illustrate the efficacy of the proposed algorithm.

## [03580] Linearized Inverse Potential Problems at a High Frequency

**Format :** Talk at Waseda University

**Author(s) :** Boxi XU (Shanghai University of Finance and Economics)

**Abstract :** We investigate the recovery of the potential function from many boundary measurements at a high frequency for linear or nonlinear equations. By considering such a linearized form, we obtain Hölder type stability which is a big improvement over logarithmic stability in low frequencies. Increasing stability bounds for these coefficients contain a Lipschitz term with a factor growing polynomially in terms of the frequency, a Hölder term, and a logarithmic term that decays with respect to the frequency as a power. Based on the linearized problem, a reconstruction algorithm is proposed aiming at the recovery of sufficiently many Fourier modes of the potential function. By choosing the high frequency appropriately, the numerical evidence sheds light on the influence of the growing frequency and confirms the improved

resolution.

This is the joint work with Prof. Victor Isakov, Prof. Shuai Lu, Prof. Mikko Salo, and Mr. Sen Zou.

## [03600] An Embedding Method for Hyperbolic Conservation Laws on Implicit Surfaces

**Format :** Talk at Waseda University

**Author(s) :** Chun Kit Hung (The Hong Kong University of Science and Technology)Shingyu Leung (The Hong Kong University of Science and Technology)

**Abstract :** In this talk, we will present a novel embedding method for solving scalar hyperbolic conservation laws on surfaces. The proposed method represents the interface implicitly through the zero-level set of its signed distance function and introduces a pushforward operator to extend the surface flux function to neighboring level surfaces. By solving an extended conservation law in a tubular neighborhood of the interface, it has been proven that the solution is the constant-normal extension of the surface conservation law. Numerical examples will be presented to demonstrate the accuracy and performance of the proposed method.

## [00353] Interpretable constrained tensor decompositions: models, algorithms, efficient implementations and applications

**Session Time & Room :**

00353 (1/3) : 3C (Aug.23, 13:20-15:00) @G306

00353 (2/3) : 3D (Aug.23, 15:30-17:10) @G306

00353 (3/3) : 5B (Aug.25, 10:40-12:20) @E803

**Type :** Proposal of Minisymposium

**Abstract :** Tensor decompositions are a fundamental tool in the data sciences for extracting interpretable patterns, removing or reducing noise, and providing reduced-dimension or low-complexity models for tensor data. In recent years, significant progress has been made to propose and understand new constrained tensor models to aid in interpretability or to satisfy known constraints on the data. In this minisymposium, we present some of the state-of-the-art approaches to interpretable constrained tensor decompositions, including efficient inference algorithms with convergence guarantees, efficient implementations of these algorithms compatible with modern hardware, and application of these models to challenging data analysis problems across several domains.

**Organizer(s) :** Axel Marmoret, Daniel M. Dunlavy, Jeremy E. Cohen

**Classification :** 15Axx, 65Kxx, 68-XX, Tensor decompositions

**Minisymposium Program :**

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00353 (1/3) : 3C @G306 [Chair: Daniel Dunlavy]

## [03825] Implicit balancing in penalized low-rank approximations

**Format :** Talk at Waseda University

**Author(s) :** Jeremy E. Cohen (CREATIS, CNRS)

**Abstract :** Tensor decompositions are an important tool in machine learning, particularly due to their interpretability which makes them well-adapted to solving inverse problems for a wide range of applications. Additional constraints and penalizations are often imposed to enhance the interpretability of these models. Because of scale-invariance in tensor decompositions, one may show that adding regularization terms, which are scale-dependent, induces an implicit balancing of the factor matrices. By explicitly imposing balancing during an optimization algorithm, I show that it is possible to improve the precision and speed of that algorithm for both nonnegative PARAFAC and Tucker decompositions.

## [02791] Hierarchical and neural nonnegative tensor factorizations

**Format :** Online Talk on Zoom

**Author(s) :** Jamie Haddock (Harvey Mudd College)Joshua Vendrow (Massachusetts Institute of Technology)Deanna Needell (University of California, Los Angeles)

**Abstract :** Nonnegative matrix factorization (NMF) has found many applications including topic modeling and document analysis. Hierarchical NMF (HNMF) variants are able to learn topics at various levels of granularity and

part\_1

illustrate their hierarchical relationship. Recently, nonnegative tensor factorization (NTF) methods have been applied in a similar fashion in order to handle data sets with complex, multi-modal structure. Hierarchical NTF (HNTF) methods have been proposed, however these methods do not naturally generalize their matrix-based counterparts. Here, we propose a new HNTF model which directly generalizes a HNMF model special case, and provide a supervised extension. Our experimental results show that this model more naturally illuminates the topic hierarchy than previous HNMF and HNTF methods. We also describe training methods for hNTF models built upon a neural network structure.

## [03781] Nonnegative canonical tensor decomposition with linear constraints: nnCANDELINC

**Format :** Talk at Waseda University

**Author(s) :** Derek DeSantis (Los Alamos National Labs)Boian Alexandrov (Los Alamos National Labs)Gianmarco Manzini (Los Alamos National Labs)Erik Skau (Los Alamos National Labs)

**Abstract :** Nonnegative tensor factorization produces sparse and easily understandable latent features. However, the Canonical Polyadic Decomposition (CPD) struggles with tensors that have rank deficient factors. The PARALIND algorithm addresses this for real-valued tensors by first computing a Tucker decomposition (TD) and then performing a CPD on the TD core to extract latent features. This work explores the theory behind the nonnegative version of PARALIND. We demonstrate nnPARALIND on several real and synthetic examples, highlighting its sensitivity and discussing when it can be applied.

## [04213] Joint Data Fusion and Blind Unmixing using Nonnegative Tensor Decomposition

**Format :** Online Talk on Zoom

**Author(s) :** Clémence Prévost (University of Lille, CNRS Centrale Lille, UMR 9189 CRISTAL F-59000 Lille, France)Valentin Leplat (Skoltech Center for Artificial Intelligence Technology (CAIT) Moscow, Russia)

**Abstract :** We present a new method for solving hyperspectral super-resolution and spectral unmixing of the unknown super-resolution image. Our method relies on (1) the nonnegative block-term decomposition, (2) joint tensor factorization with multiplicative updates, and (3) the formulation of optimization problems with the beta-divergence. We propose a family of algorithms, adaptable to various noise statistics. Experiments show that our approach competes favorably with state-of-the-art for solving both problems for various noise statistics.

, blockterm

decomposition, -divergence, blind spectral unmixing,  
hyperspectral super-resolution.

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00353 (2/3) : 3D @G306 [Chair: Jeremy E. Cohen]

## [04776] A quadratically convergent proximal algorithm for nonnegative tensor decomposition

**Format :** Talk at Waseda University

**Author(s) :** Nico Vervliet (KU Leuven)Andreas Themelis (Kyushu University)Panagiotis Patrinos (KU Leuven)Lieven De Lathauwer (KU Leuven)

**Abstract :** The canonical polyadic decomposition is key in a variety of applications in signal processing and data analysis. While this decomposition is unique under mild conditions, including prior knowledge such as nonnegativity often helps to interpret the components. We derive a proximal Gauss-Newton-type algorithm for nonnegative tensor factorization. We show global convergence to local minima, as well as a  $Q$ -quadratic convergence rate to global optima in the exact case.

## [03079] PARAFAC2-based coupled matrix and tensor factorizations with constraints

**Format :** Online Talk on Zoom

**Author(s) :** Carla Schenker Xiulin Wang (Dalian University of Technology)Evrim Acar (Simula Metropolitan Center for Digital Engineering)

**Abstract :** There is an emerging need to jointly analyze time-evolving data sets together with static data in many areas such as social networks and omics data analysis. PARAFAC2-based coupled matrix and tensor factorizations are a promising approach in that direction, since PARAFAC2 is capable of capturing time-evolving patterns. We present a flexible algorithmic framework for such factorizations which facilitates linear couplings and various constraints on all modes, including the evolving mode in the PARAFAC2 model.

## [03791] Constrained Tucker Decompositions and Conservation Principles for Direct Numerical Simulation Data Compression

**Format :** Talk at Waseda University

**Author(s) :** Daniel Dunlavy (Sandia National Laboratories)

**Abstract :** Low-rank tensor decompositions applied to numerical simulation data for compression and reduced-order modeling often focus only on minimizing global error norms between data and the low-rank model. We present an approach for computing goal-oriented low-rank tensor decompositions that incorporates problem-specific quantities of interest (QoIs) through general nonlinear constraints added to the tensor model loss function. Results for compression of direct numerical simulation data from multiple applications are presented to demonstrate the utility of this approach.

## [03819] Incremental Nonnegative Tucker Decomposition with Block-coordinate Descent and Recursive Approaches

**Format :** Online Talk on Zoom

**Author(s) :** Rafal Zdunek (Wroclaw University of Science and Technology) Krzysztof Fornal (Wroclaw University of Science and Technology)

**Abstract :** We extend the standard model of Nonnegative Tucker decomposition (NTD) to an incremental or online version, assuming volatility of observed multi-way data along one mode. Two computational approaches are proposed: one is based on the recursive update model, and the other uses the concept of the block-Kaczmarz method. The experimental results performed on various datasets and streaming data demonstrate high efficiency of both algorithmic approaches with respect to the baseline NTD methods.

00353 (3/3) : 5B @E803 [Chair: Daniel Dunlavy]

## [05162] Speeding up Nonnegative Low-rank Approximations with Parallelism and Randomization.

**Format :** Online Talk on Zoom

**Author(s) :** Koby Hayashi (Georgia Institute of Technology)

**Abstract :** Many algorithms for constrained matrix and tensor factorization follow an alternating updating scheme. In such a scheme, the factor matrices are updated one at a time using some update rule. Computationally many update rules require the same bulk computations. That is the most expensive parts of the computations needed to perform an update are shared between update rules. Using this observation, we design a Framework for Alternating Updating NMF and NTF (FAUN). FAUN defines the bulk computations needed throughout an AU type algorithm allowing us to focus on optimizing these computations for multiple methods. Based on this we implement a distributed, highly parallel code called PLANC which optimizes computation and communication and allows for the use of various updating rules such as Hierarchical Least Squares, Nonnegative Least Squares, ADMM, Nesterov updates, etc... More recently we have explored the use of randomization in FAUN. As in the parallel case we can largely decouple the randomized aspects of the algorithms from the update rules.

## [03142] A probabilistic nonnegative tensor factorization method for tumor microenvironment analysis

**Format :** Online Talk on Zoom

**Author(s) :** Neriman Tokcan (University of Massachusetts Boston)

**Abstract :**

The tumor microenvironment (TME) comprises the intricate environment surrounding cancer cells, such as stromal, immune, and extracellular elements. We have devised a probabilistic non-negative tensor factorization approach to model the TME of Hodgkin Lymphoma. We have also incorporated a statistical pipeline to produce robust and biologically relevant factors. Our methodology will enhance our understanding of the TME by identifying cellular heterogeneity and intrinsic pathways driving tumor growth and immune evasion.

## [03182] Scalable symmetric Tucker tensor decomposition

**Format :** Online Talk on Zoom

**Author(s) :** Ruhui Jin (UW-Madison) Joe Kileel (UT-Austin) Tamara Kolda (MathSci.ai) Rachel Ward (UT-Austin)

**Abstract :** We study the best low-rank Tucker decomposition of symmetric tensors. The motivating application is in decomposing higher-order multivariate moments, which has special structure and is important to various data science problems. We advocate for a straightforward projected gradient descent (PGD) method and the higher-order eigenvalue part\_1

decomposition (HOEVD) approximation as computation schemes. Most importantly, we develop scalable adaptations of the basic PGD and HOEVD methods to decompose sample moment tensors. With the help of implicit and streaming technique, we evade the overhead cost of building and storing the moment tensor. Such reductions make computing the Tucker decomposition realizable for large data instances in high dimensions. Numerical experiments demonstrate the efficiency of the algorithms and the applicability of moment tensor decompositions to real-world datasets. Finally we study the convergence on the Grassmannian manifold and prove that the update sequence derived by the PGD solver achieves first and second-order criticality

## [02021] A tensor factorization model of multilayer network interdependence

**Format :** Online Talk on Zoom

**Author(s) :** Izabel Aguiar (Stanford University)Dane Taylor (University at Buffalo the State University of New York)Johan Ugander (Stanford University)

**Abstract :** We use the nonnegative Tucker decomposition (NNTuck) with KL-divergence as an expressive factor model for multilayer networks that naturally generalizes existing methods for stochastic block models of multilayer networks. The NNTuck provides a factor-based perspective on layer dependence, enabling linear-algebraic techniques for analyzing dependence in specific layers. We propose a definition of layer dependence based on a likelihood ratio test and evaluate the NNTuck in synthetic and real-world data.

## [00356] Recent progress in variational problems with nonlocality

**Session Time & Room :**

00356 (1/2) : 3C (Aug.23, 13:20-15:00) @F401

00356 (2/2) : 3D (Aug.23, 15:30-17:10) @F401

**Type :** Proposal of Minisymposium

**Abstract :** This minisymposium will discuss some recent developments in the analysis of variational problems from science and engineering in which nonlocal interactions have a pronounced effect. Examples will include geometric variational problems with long-range repulsion, topologically non-trivial spin configurations in magnetic materials, long-range interactions in phase transitions, capillary theory and theory of dislocations.

**Organizer(s) :** Cyrill Muratov, Matteo Novaga, Valeriy Slastikov

**Classification :** 49J99, 35R11, 35B65, 53E99

**Minisymposium Program :**

00356 (1/2) : 3C @F401 [Chair: Matteo Novaga]

## [03768] Nonlocal capillarity theory

**Format :** Online Talk on Zoom

**Author(s) :** Enrico Valdinoci (University of Western Australia)

**Abstract :** We describe some recent results motivated by a nonlocal theory of capillarity, as related to the formation of droplets due to long-range interaction potentials. We will discuss the notion of contact angle in this setting, considering a nonlocal version of the classical Young's Law, together with some regularity and asymptotic properties.

## [03751] Skyrmiion theory in magnetic thin films: the role of non-local magnetic dipolar interaction

**Format :** Talk at Waseda University

**Author(s) :** Anne Bernand-Mantel Cyrill Muratov (University of Pisa)Theresa Simon (Muenster University)Valeriy Slastikov (Bristol University)

**Abstract :** Compact magnetic skyrmion are potential bit-encoding states for spintronic memory and logic applications that have been the subject of a rapidly growing number of studies in recent years. We will present our recent work where we used rigorous mathematical analysis to develop a skyrmion theory that takes into account the full dipolar energy in the thin film regime and provides analytical formulas for compact skyrmion radius, rotation angle and energy.

## [05516] Long-range phase transition equations

**Format :** Talk at Waseda University

**Author(s) :** Serena Dipierro (University of Western Australia)

**Abstract :** In this talk, we will review recent results on long-range phase transitions.

## [04003] A distributional approach to nonlocal curvature motions

**Format :** Online Talk on Zoom

**Author(s) :** Massimiliano Morini (University of Parma)

**Abstract :** After reviewing the new distributional approach recently developed to provide a well-posed formulation of the crystalline mean curvature flow, we show how to extend it to some nonlocal motions. Applications include the fractional mean curvature flow and the Minkowski flow; i.e., the geometric flow generated by the  $(n-1)$ -dimensional Minkowski pre-content. This is a work in collaboration with F. Cagnetti (University of Sussex) and D. Reggiani (Scuola Superiore Meridionale).

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00356 (2/2) : 3D @F401 [Chair: Cyrill Muratov]

## [03830] The elastica functional as the critical Gamma-limit of the screened Gamow model

**Format :** Talk at Waseda University

**Author(s) :** Theresa Simon (University of Münster)Cyrill Muratov (University of Pisa)Matteo Novaga (University of Pisa)

**Abstract :** I will consider the large mass limit of a nonlocal isoperimetric problem in two dimensions with screened Coulomb repulsion. In this regime, the nonlocal interaction localizes on the boundary of the sets. It turns out that in the case of exactly cancelled surface area, the problem changes from length to curvature minimization: The next-order Gamma limit is given by the elastica functional, i.e., the integral over the squared curvature over the boundary.

## [04447] Minimisers of anisotropic Coulomb energies in 3d

**Format :** Talk at Waseda University

**Author(s) :** Lucia Scardia (Heriot-Watt University)

**Abstract :** Nonlocal energies are continuum models for large systems of particles with long-range interactions. Under the assumption that the interaction potential is radially symmetric, several authors have investigated qualitative properties of energy minimisers.

But what can be said in the case of anisotropic kernels?

I will present some results and partial answers in this direction obtained in a long-standing collaboration with Maria Giovanna Mora and Luca Rondi, and with Jose' Antonio Carrillo, Joan Mateu and Joan Verdera.

## [03755] Minimal partitions for local and nonlocal energies

**Format :** Talk at Waseda University

**Author(s) :** Annalisa Cesaroni (University of Padova)

**Abstract :** The Kelvin problem, posed by Lord Kelvin in 1887, is the problem of finding a partition of  $\mathbb{R}^3$  into cells of equal volume, so that the total area of the surfaces separating them is as small as possible.

I will discuss some related problems in  $\mathbb{R}^n$ , in particular the problem of finding the foam whose cell minimizes a general perimeter functional among all periodic partitions given by lattice tilings. Moreover I will present some qualitative results in low dimension.

## [03839] Asymptotics of phase field models for crystal defects

**Format :** Talk at Waseda University

**Author(s) :** Adriana Garroni (Sapienza, University of Rome)Sergio Conti (University of Bonn)Stefan Mueller (University of Bonn)

**Abstract :** We consider Nabarro Peierls type model for line defects in crystals. We study the asymptotics in scaling regime which allows for the number of dislocations to diverge and results, in the limit as the lattice spacing tends to zero, in a macroscopic model for plasticity where the relevant variable is a diffuse quantity that represents the dislocation density.

# [00357] Topics at the Interface between Applied mathematics and Microeconomics

**Session Time & Room :** 2E (Aug.22, 17:40-19:20) @D501

**Type :** Proposal of Minisymposium

**Abstract :** Traditionally, economic models were easier to understand in the context of economics. Still, recent advances in mathematical methods, particularly in applied mathematics and computer science, enable a more realistic and intuitive approach to economic phenomena. This session will present recent research on how economic theory relates to applied mathematics.

**Organizer(s) :** Yujiro Kawasaki, Kuninori Nakagawa

**Classification :** 91A28, 91B24, 91B44, 91B80, Game Theory, Economics, Data Science

**Minisymposium Program :**

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00357 (1/1) : 2E @D501 [Chair: Kuninori Nakagawa]

## [01659] Commitment games with mutual interferences

**Format :** Talk at Waseda University

**Author(s) :** Ryosuke Ishii (Shimonoseki City University)

**Abstract :** As a stabilization device of an efficient outcome that is not an equilibrium as it now stands outcome, commitments have been assembled in game theory literature. Earlier studies suggest that efficient outcomes are subgame perfect if a game is expressed by an extensive form with a perfect information. However, an outcome of a game with simultaneous moves is not always efficient, most often happen when players face a prisoners' dilemma like situation. This research considers a game in which players can determine success or failure of other players' commitment one another. The result is similar to a Folk Theorem. That is, players can achieve efficiency in prisoners' dilemma games. In contrast, the worst mixed equilibrium outcome is subgame perfect in coordination games.

## [01666] Equilibria in a spatial competition with uninformed consumers

**Format :** Talk at Waseda University

**Author(s) :** Kuninori Nakagawa (University of Hyogo)Shinnosuke Kawai (Shizuoka University)

**Abstract :** We extend a model that analyses explicit product differentiation in Varian's model of sales using a one-dimensional spatial competition framework. We study the price equilibrium in the case of a uniform distribution of informed consumers. We give examples of price game equilibria given pairs of locations and discuss the difficulties associated with computing equilibria.

## [01655] Gradient flows in travelers' visitation network: comparison with centrality indices

**Format :** Online Talk on Zoom

**Author(s) :** Yujiro Kawasaki (Nagoya Institute of Technology)Kenta Kojima (Kansai University)Jun'ichi Miki (Tohoku University of Community Service and Science)

**Abstract :** The Hodge decomposition defined on discrete graphs has been applied to analyzing network structures related to various economic activities. We use the travel data of tourists visiting a regional city in Japan to examine the effectiveness of the Hodge decomposition on the network of tourist movements between sightseeing spots. By employing centrality indices together, we provide robust trends of tourist visits and, thus, the function of each sightseeing spot.

## [01678] Information Design and Pre-trade Investment

**Format :** Online Talk on Zoom

**Author(s) :** Keiichi Kawai (Keio University)

**Abstract :** We analyze a bilateral trade model where, after the buyer makes a take-it-or-leave-it offer, the seller can make a costly investment which stochastically increases the value of the good to both players. The seller partially learns about the investment outcome before deciding whether to trade. The efficiency of the outcome is undermined by both the adverse selection problem in trade, and the seller's moral hazard in investment. We identify all second-best outcomes.

# [00372] Recent advances on computational wave propagation

## **Session Time & Room :**

00372 (1/3) : 3D (Aug.23, 15:30-17:10) @D404

00372 (2/3) : 3E (Aug.23, 17:40-19:20) @D404

00372 (3/3) : 4C (Aug.24, 13:20-15:00) @D404

**Type :** Proposal of Minisymposium

**Abstract :** This mini-symposium is organized to provide a forum for fellow researchers working on numerical methods for wave propagation problems to present and discuss their recent advances and achievements. Topics to be covered include but not limited to: FDTD methods, finite element methods, spectral methods, multiscale methods, novel techniques for metamaterials and graphene.

**Organizer(s) :** Jichun Li, Nathan Gibson

**Classification :** 78-10, 65Nxx, 35Mxx, 35Qxx, Computational Electromagnetics; Maxwell's Equations; Wave Propagation

## **Minisymposium Program :**

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00372 (1/3) : 3D @D404 [Chair: Jichun Li]

## [01429] Analysis and simulation of carpet cloak model with metamaterials

**Format :** Talk at Waseda University

**Author(s) :** Jichun Li (University of Nevada Las Vegas)

**Abstract :** This talk is concerned about a time-domain carpet invisibility cloak model. Here we consider two new finite element schemes to solve it. Stability and optimal error estimates are proved for both schemes. Numerical results are presented to support our analysis and demonstrate the cloaking phenomenon.

## [01639] Edge elements on nonaffine quadrilateral and hexahedral grids for Maxwell eigenproblem

**Format :** Talk at Waseda University

**Author(s) :** HUOYUAN DUAN (Wuhan University, School of Mathematics and Statistics)

**Abstract :** Most of the edge elements on nonaffine quadrilateral and hexhaedral grids do not satisfy the so-called discrete compactness property. Consequently, they generate spurious eigenmodes and are not spectral correct. We propose some new finite element methods for Maxwell eigenproblems so that all the edge elements on nonaffine quadrilateal and hexhaedral grids are spurious-free and spectral correct. The new methods have been confirmed by theory and numerics.

## [01856] Deriving consistent surface fields for compatible FETD discretizations of Maxwell's equations

**Format :** Talk at Waseda University

**Author(s) :** Duncan McGregor (Sandia National Laboratories)

**Abstract :** The coupling of electromagnetic energy to a cable is a critical quantity of interest in some engineering applications. These cables can be modelled as internal boundaries with a perfect electric conductor condition. An intuitive method is a loop integral of the magnetic field around the cable. This leads to physical and mathematical concerns. As such, we use Dirichlet-to-Neumann map to compute surface currents. We will describe our method and present numerical results.

## [01860] FDTD Method With Explicit Non-Iterative and Second Order Treatment for Kerr Nonlinearities

**Format :** Talk at Waseda University

**Author(s) :** Jinjie Liu (Delaware State University)

**Abstract :** In this talk, we introduce a new explicit non-iterative FDTD algorithm for solving Maxwell's equations in nonlinear Kerr media. The FDTD method is a widely used numerical technique for solving Maxwell's equations in complex media. Our method balances accuracy and computational cost, offering similar accuracy to Newton's iterative method but at a lower computational expense. The effectiveness of our method is demonstrated by its quadratic

convergence rate, as well as several numerical examples such as simulations of four-wave mixing and soliton propagation.

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00372 (2/3) : 3E @D404 [Chair: Nathan Gibson]

## [02077] Harnessing the Power of Exascale Computing for Microelectronics Modeling

**Format :** Talk at Waseda University

**Author(s) :** Zhi Jackie Yao (Lawrence Berkeley National Lab)Revathi Jambunathan (Lawrence Berkeley National Lab)Andy Nonaka (Lawrence Berkeley National Lab)Prabhat Kumar (Lawrence Berkeley National Lab)Saurabh Sawant (Lawrence Berkeley National Lab)

**Abstract :** As the era of Moore's law comes to a close, there has been a surge in the development of microdevices that involve more complex physical interactions than conventional electromagnetic waves and single-phase materials. However, gaining a deeper understanding of these interactions has been hindered by the significant disparity in time and length scales and a lack of effective modeling techniques.

To address these challenges, we have developed ARTEMIS, a scalable simulation tool that harnesses the power of GPU-based supercomputing systems to model next-generation microelectronic devices, including electronic, spintronic, superconducting, and ferroelectric systems. ARTEMIS leverages the developments of two Exascale Computing Projects and supports dispersive material properties, user-defined excitations and boundary conditions, and heterogeneous physical coupling. Specifically, with its micromagnetics module, ARTEMIS is suitable for nonlinear spintronic applications and can be used as a device-level design and optimization tool.

This new approach also provides a path to understanding and developing fully integrated electronic systems that go beyond the capabilities of traditional semiconductor technologies. ARTEMIS will enable a broader exploitation of new materials and provide new mechanisms for everything from low-power computing to high-efficiency microwave components, contributing to the development of next-generation architectures.

## [02080] Simulating Time Domain Electromagnetic Waves on a Differentiable Programming Platform

**Format :** Talk at Waseda University

**Author(s) :** Yanyan Hu (University of Houston)Yuchen Jin (University of Houston)Xuqing Wu (University of Houston)Jiefu Chen (University of Houston)

**Abstract :** A trainable theory-guided recurrent neural network (RNN) equivalent to finite-difference-time-domain (FDTD) method is designed to formulate electromagnetic propagation, solve Maxwell's equations, and the inverse problem on differentiable programming platform PyTorch. For forward modeling, the computation efficiency is substantially improved. The inverse problem can be solved by setting the trainable weights of RNN as the material-related parameters and network training. Numerical results demonstrate the effectiveness and efficiency of the method for forward and inverse electromagnetic modeling.

## [02117] Iterative two-level algorithm for nonsymmetric or indefinite problems

**Format :** Talk at Waseda University

**Author(s) :** Ming Tang (South China Normal University)Xiaoqing Xing (South China Normal University)Ying Yang (Guilin University of Electronic Technology)Liuqiang Zhong (South China Normal University)

**Abstract :** In this talk, some new iterative two-level algorithms are designed and analyzed for solving the finite element discretization for nonsymmetric or indefinite elliptic/Maxwell problems. The two-level methods use only the same coarse spaces as the traditional two-grid algorithm, but its "fine spaces" use the higher order finite element space under the coarse grid. Therefore, the iterative two-level algorithm only need one grid and achieve the same convergence order of the traditional two-grid algorithms. At last. Numerical experiments are implemented to support the theoretical results, especially, the computational cost of two-level algorithms are lower to achieve the same convergence order for traditional two-grid algorithms.

## [01863] Analysis and application of FEMs for Ziolkowski's PML model

**Format :** Talk at Waseda University

**Author(s) :** Li Zhu (Portland State University)Jichun Li (University of Nevada Las Vegas)

**Abstract :** Perfectly Matched Layer PML technique is an effective tool proposed by Berenger to solve a wave propagation problem in unbounded domain without reflections. Here we are interested in the Ziolkowski PML reformulated in an integro-differential form, We introduce two novel FEMs for solving this equivalent PML model. Stability and convergence analysis are established for both schemes. Numerical results are presented to support our analysis and demonstrate the wave absorption effectiveness of this PML.

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## [02737] Highly Efficient Iterative Method with High Order ABC for Acoustic Scattering

**Format :** Talk at Waseda University

**Author(s) :** Vianey Roman Villamizar (Brigham Young University)Tahsin Khajah (University of Texas at Tyler)Jonathan Hale (University of Wisconsin)

**Abstract :** In this paper, we have developed a highly efficient numerical method for acoustic multiple scattering. This novel method consists of a high order local absorbing boundary condition combined with an isogeometric finite element and finite differences methods. By employing high order NURB basis, a globally high order method results. In our numerical experiments, we obtain errors close to machine precision by appropriate implementation of p- and h-refinement. We include numerical results which demonstrate the improved accuracy and efficiency of this new formulation compared with similar methods.

## [02916] The effect normal electric fields on the flow structure beneath waves

**Format :** Talk at Waseda University

**Author(s) :** Roberto Ribeiro Santos Junior (Universidade Federal do Paraná)Marcelo V. Flamarion (Rural Federal University of Pernambuco)Tao Gao (University of Essex)Alex Doak (University of Bath)

**Abstract :** Waves with constant vorticity and electrohydrodynamics flows are two topics in fluid dynamics that have attracted much attention from scientists for both the mathematical challenge and their industrial applications. The coupling of electric fields and vorticity is of significant research interest. In this talk, we present numerical results on the effect of normal electric fields on the flow structure beneath periodic and solitary rotational waves. By using a combination of conformal mapping techniques and pseudo-spectral numerical methods, we show how variations in voltage potential can affect particle trajectories and the pressure within the bulk of the fluid

## [00378] Mathematical Methods in System Reliability

**Session Time & Room :**

00378 (1/2) : 2C (Aug.22, 13:20-15:00) @D408

00378 (2/2) : 2D (Aug.22, 15:30-17:10) @D408

**Type :** Proposal of Minisymposium

**Abstract :** System reliability is a measure of the performance of an engineering system. High-tech industrial processes increase in complexity and at the same time, system failures are having more significant impacts on society than ever before. Hence, the importance of reliability in modern engineering processes, can hardly be overstated.

The reliable performance of complex systems depends on the performance of their components and the system's structure. In recent years, advanced statistical, probabilistic and algebraic methods and techniques have been applied to system reliability. This minisymposium brings together recent developments of mathematical methods applied to industrial system reliability.

**Organizer(s) :** Fatemeh Mohammadi, Eduardo Sáenz-de-Cabezón, Henry Wynn

**Classification :** 90B25, 62N05, 68M15, Reliability Theory

**Minisymposium Program :**

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00378 (1/2) : 2C @D408 [Chair: Christian Tanguy]

## [01347] Domination and multistate systems

**Format :** Talk at Waseda University

**Author(s) :** Arne Bang Huseby (University of Oslo)

**Abstract :** Domination functions has been studied extensively in the context of binary systems, where the structure function is a sum of products of the component states, and with coefficients given by the domination function. Using matroid theory, properties of the domination function can be derived. We generalise these results to multistate systems. The domination is determined by the poset generated by the minimal paths, and two systems with isomorphic posets also have the same domination function.

## [01419] Mathematical analysis of the reliability of stable systems

**Format :** Talk at Waseda University

**Author(s) :** Eduardo Sáenz-de-Cabezón (University of La Rioja)

**Abstract :** One of the main characteristics of coherent systems is redundancy. In this talk we define stability as a way to encode redundancy in a way that generalizes well known systems like k-out-of-n and variants. We furthermore provide a complete algebraic analysis of the reliability of these systems and design based on stability.

## [01422] Algebraic probability: the case of system reliability

**Format :** Online Talk on Zoom

**Author(s) :** Henry Wynn (London School of Economics)

**Abstract :** Algebra arises in probability because of additivity over set disjointness and multiplication with independence. With systems such as those in causal analysis, data analysis and reliability we can have rich algebraic structures. In reliability, under coherence, failure patterns give rise to monomial ideals and from there Betti numbers and Hilbert series lead to efficient identities and bounds for failure probabilities. Structures such as mixed series-parallel systems and multi state systems have special features.

## [01425] Algebraic analysis of importance measures of coherent systems

**Format :** Online Talk on Zoom

**Author(s) :** Patricia Pascual-Ortigosa (University of La Rioja)Eduardo Sáenz-de-Cabezón (University of La Rioja)Rodrigo Iglesias (University of La Rioja)

**Abstract :** The aim of this talk is to do an analysis of importance measures of coherent systems using an algebraic approach.

First of all, we introduce what importance measures are, providing a classification of them and some background for all of them. Then, we will show how Algebra can help us to study structural measures of importance of coherent systems. Finally, we present some examples explaining the advantages and disadvantages of this approach.

00378 (2/2) : 2D @D408 [Chair: Eduardo Sáenz-de-Cabezón]

## [01455] New exactly solvable architecture for system reliability and safety

**Format :** Talk at Waseda University

**Author(s) :** Christian Tanguy (Orange)

**Abstract :** Network reliability is a crucial performance index for telecommunication operators. In the general case, the calculation of the two-terminal reliability is known to be #P-complete, even for identical links and perfect nodes of the network's underlying graph. Exact solutions have nonetheless been found for a few recursive architectures. We present a new example of such an architecture, which could be of interest to reliability practitioners and graph theorists.

## [01469] Application of Logic Differential Calculus in Reliability Analysis

**Format :** Online Talk on Zoom

**Author(s) :** Michal Mrena (University of Zilina)

**Abstract :** Logic differential calculus – specifically logic derivatives – provides an efficient way to investigate the reliability of systems described by a structure function. The structure function captures the topology of the system and the derivatives describe the behavior of the system when the state of a component changes. Consequently, they allow us to calculate importance measures for individual components. In this contribution, we present a comprehensive framework for the evaluation of various system reliability characteristics.

## [03092] Stochastic comparisons of coherent systems with active redundancy at component level and system level

**Format :** Talk at Waseda University

**Author(s) :** Pradip Kundu (XIM University, Bhubaneswar)Arindam Panja (Indian Statistical Institute)Biswabrata Pradhan (Indian Statistical Institute)

**Abstract :** An effective way to increase system reliability is to use redundancies (spares) into the systems. In this paper, we derive sufficient conditions under which a coherent system with a set of active redundancy at the component level or the system level provides better system reliability than that of the system with another set of redundancy, with respect to some stochastic orders. We have derived the results for the component lifetimes following accelerated life (AL) model.

# [00379] Numerical techniques for coarse-graining, model reducing and simulation of complex physical systems

## **Session Time & Room :**

00379 (1/4) : 1C (Aug.21, 13:20-15:00) @E505

00379 (2/4) : 1D (Aug.21, 15:30-17:10) @E505

00379 (3/4) : 1E (Aug.21, 17:40-19:20) @E505

00379 (4/4) : 2C (Aug.22, 13:20-15:00) @E505

## **Type :** Proposal of Minisymposium

**Abstract :** The simulation of complex physical systems for prediction and control requires robust, efficient mathematical modeling and numerical algorithms, as the problem size and time scales of interest in many applications are typically beyond which can be simulated directly. In recent years, a wealth of new techniques and algorithms have been developed to help reduce problem size/dimension and accelerate the accurate simulation of various classes of physical observables while quantifying the uncertainty of the resulting predictions made. Examples of such techniques include Coarse-Grained Molecular Dynamics, Nonlocal Theories of Mechanics, Time Accelerated Dynamics, Hyperdynamics, Space-Time Homogenization, and so on. These techniques and numerical algorithms have made successful applications in a diverse range of models.

In view of the wide range of applicability of these algorithms and the ideas which lie behind them, this minisymposium seeks to bring together both theoreticians and practitioners who study and use numerical simulations for a range of practical scientific problems, aiming to facilitate discussion and two-way dissemination of ideas across disciplinary and topical boundaries.

**Organizer(s) :** Yanlai Chen, Xingjie Helen Li, Xiaochuan Tian, Yue Yu

**Classification :** 65AXX, 00A69, 37NXX

## **Minisymposium Program :**

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00379 (1/4) : 1C @E505 [Chair: Yanlai Chen]

## [02156] Ahyper-reduced MAC scheme for the parametric Stokes and Navier-Stokes equations

### **Format :** Talk at Waseda University

**Author(s) :** Lijie Ji (Shanghai Jiao Tong University)

**Abstract :** The classical reduced basis method is popular due to an offline-online decomposition and a mathematically rigorous a posterior error estimator which guides a greedy algorithm offline. For nonlinear and nonaffine problems, hyper reduction techniques have been introduced to make this decomposition efficient. However, they may be tricky to implement and often degrade the offline and online computational efficiency. In this talk, I will introduce an adaptive enrichment strategy for R2-ROC rendering it capable of handling parametric fluid flow problems. Tests on lid-driven cavity and flow past a backward-facing step problems demonstrate its high efficiency, stability and accuracy.

## [02166] Hybrid Projection Methods for Solution Decomposition in Large-scale Bayesian Inverse Problems

### **Format :** Talk at Waseda University

**Author(s) :** Jiahua Jiang (University of Birmingham) Julianne Chung (Emory University) Arvind Krishna Saibaba (North Carolina State University) Scot Miller (John Hopkins )

**Abstract :** We develop hybrid projection methods for computing solutions to large-scale inverse problems, where the solution represents a sum of different stochastic components. Such scenarios arise in many imaging applications (e.g., anomaly detection in atmospheric emissions tomography) where the reconstructed solution can be represented as a combination of two or more components and each component contains different smoothness or stochastic properties. In a deterministic inversion or inverse modeling framework, these assumptions correspond to different regularization terms for each solution in the sum. Although various prior assumptions can be included in our framework, we focus on the scenario where the solution is a sum of a sparse solution and a smooth solution. For computing solution estimates, we develop hybrid projection methods for solution decomposition that are based on a combined flexible and generalized Golub-Kahan processes. This approach integrates techniques from the generalized Golub-Kahan bidiagonalization and the flexible Krylov methods. The benefits of the proposed methods are that the decomposition of the solution can be

done iteratively, and the regularization terms and regularization parameters are adaptively chosen at each iteration. Numerical results from photoacoustic tomography and atmospheric inverse modeling demonstrate the potential for these methods to be used for anomaly detection.

## [02484] A reduced basis method for the parametrized Monge-Ampere equation

**Format :** Talk at Waseda University

**Author(s) :** Shijin Hou (University of Science and Technology of China)

**Abstract :** In this talk, we first introduce a highly efficient solver for the parameterized optimal mass transport problem by adapting the reduced residual reduced over-collocation approach to the parameterized Monge-Ampère equation. This new reduced basis technique allows us to handle the strong and unique nonlinearity pertaining to the Monge-Ampère equation achieving online efficiency. After that, several numerical tests will be presented to demonstrate the accuracy and high efficiency of our reduced solver.

## [04068] Novel Reduced Basis Method for Radiative Transfer Equation

**Format :** Talk at Waseda University

**Author(s) :** ZHICHAO PENG (Michigan State University)Yanlai Chen (University of Massachusetts Dartmouth)Yingda Cheng (Michigan State University)Fengyan Li (Rensselaer Polytechnic Institute)

**Abstract :** One prominent computational challenge to simulate radiative transfer (RTE), a fundamental kinetic description of energy or particle transport through mediums affected by scattering and absorption processes, comes from the high dimensionality of the phase space. Leveraging the existence of a low-rank structure in the solution manifold induced by the angular variable in the scattering dominating regime, reduced order models are designed and tested here for the linear RTE model based on reduced basis methods.

00379 (2/4) : 1D @E505 [Chair: Xingjie Helen Li]

## [03752] Large Deviations for Model Coarse Graining

**Format :** Talk at Waseda University

**Author(s) :** Tobias Grafke (Warwick Mathematics Institute)

**Abstract :** Systems with time-scale separation allow effective model reduction via averaging and homogenization, where average effects of fluctuating degrees of freedom are as reduced dynamics. In the language of probability theory, this averaging corresponds to a law-of-large numbers, making it natural to ask about expected fluctuations and large deviations. In this talk, I will introduce developments regarding large deviations in the presence of time-scale separation for the computation of rare event probabilities in reduced models.

## [03592] Mean curvature flow as the limit of a spin system

**Format :** Talk at Waseda University

**Author(s) :** Patrick van Meurs (Kanazawa University)

**Abstract :** I will present the derivation of a continuum mean-curvature flow as a certain hydrodynamic scaling limit of a stochastic particle system (Glauber-Kawasaki) on the discrete torus in d dimensions. The particles can jump to neighboring vacant sites and there is a creation and annihilation mechanism. Our work combines techniques from probability theory (in particular the relative entropy method), numerical analysis and PDE theory.

Collaborators: T. Funaki, S. Sethuraman, K. Tsunoda.

## [04679] Model reduction methods for non-reversible multiscale dynamics: a comparison

**Format :** Talk at Waseda University

**Author(s) :** Lara Neureither (BTU Cottbus)

**Abstract :** In this talk we will compare existing coarse graining methods such as averaging, effective dynamics as well as the normal form approach among others for multiscale dynamics given by a non-reversible Ornstein-Uhlenbeck process driven by degenerate noise. We will address the following questions: which of the methods yields the best approximation to the original dynamics? What causes the differences in the approaches, if there are any?

## [04002] Model Reduction using the Koopman Operator

**Format :** Talk at Waseda University

**Author(s) :** Xiu Yang (Lehigh University)Bian Li (Lehigh University)Yi-An Ma (University of California at San Diego)J. Nathan Kutz (University of Washington)

**Abstract :** We propose the adaptive spectral Koopman (ASK) method to solve nonlinear autonomous dynamical systems. ASK leverages the spectral method and the Koopman operator to obtain the solution. Specifically, this solution is represented by Koopman operator's eigenfunctions, eigenvalues, and Koopman modes. Numerical experiments demonstrate high accuracy of ASK for solving both ordinary and partial differential equations. Using ASK as a surrogate model, we can design novel efficient uncertainty quantification methods.

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00379 (3/4) : 1E @E505 [Chair: Xiaochuan Tian]

## [04693] Machine-learning-based spectral methods for partial differential equations

**Format :** Talk at Waseda University

**Author(s) :** Panos Stinis (Pacific Northwest National Laboratory)Saad Qadeer (Pacific Northwest National Laboratory)Brek Meuris (University of Washington)

**Abstract :** We use deep neural operators to identify custom-made basis functions for constructing spectral methods for partial differential equations. The custom-made basis functions are studied both for their approximation capability and used to expand the solution of linear and nonlinear time-dependent PDEs. The proposed approach advances the state of the art and versatility of spectral methods and, more generally, promotes the synergy between traditional scientific computing and machine learning.

## [03852] Optimal control for fractional order equations

**Format :** Talk at Waseda University

**Author(s) :** Christian Glusa (Sandia National Laboratories)

**Abstract :** We consider adjoint-based optimization for control problems involving fractional-order state equations, applied to the inference of kernel parameters. We will discuss optimality conditions, error estimates and techniques to efficiently explore the parameter space and approximate gradients.

## [04163] Multi-Resolution and FVM inspired Neural Network (MuRFiV-Net) for PDE prediction

**Format :** Talk at Waseda University

**Author(s) :** Xin-Yang Liu (University of Notre Dame)Jian-Xun Wang (University of Notre Dame)

**Abstract :** Predicting physical processes requires modeling complex spatiotemporal dynamics. Traditional numerical methods are expensive in many-query tasks, while data-driven neural networks face issues of high training costs and poor generalizability. Physics-informed deep learning (PiDL) combines numerical methods and deep learning, offering a promising approach to overcome these limitations. This work proposes MuRFiV-Net, a novel PiDL architecture based on a multi-resolution mesh and finite volume method. The merit of MuRFiV-Net is demonstrated on several PDE-governed dynamic systems.

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00379 (4/4) : 2C @E505

## [00382] Stochastic control and stochastic analysis in finance and insurance

**Session Time & Room :**

00382 (1/3) : 2C (Aug.22, 13:20-15:00) @D514

00382 (2/3) : 2D (Aug.22, 15:30-17:10) @D514

00382 (3/3) : 2E (Aug.22, 17:40-19:20) @D514

**Type :** Proposal of Minisymposium

**Abstract :** Stochastic control and stochastic analysis have played core roles in quantitative finance and insurance. Newly emerging financial and risk models, trading constraints, behavioral decision making and time inconsistency issues have brought many new mathematical challenges. Some novel PDE techniques, mean field game formulation, optimal transport, deep learning and reinforcement learning have been rapidly developed in addressing these problems. The goal of this minisymposium is to provide a forum for some experts to exchange ideas and explore possible collaborations in modelling and methodologies in financial and insurance applications.

**Organizer(s) :** Xiaolu Tan, Kazutoshi Yamazaki, Xiang Yu

**Classification :** 91Gxx, 93Exx, 60XX, 90Bxx

**Minisymposium Program :**

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00382 (1/3) : 2C @D514 [Chair: Xiang Yu]

### [02210] Lévy bandits under Poissonian decision times

**Format :** Talk at Waseda University

**Author(s) :** Kazutoshi Yamazaki (University of Queensland) Jose Luis Perez (CIMAT)

**Abstract :** We consider a version of the continuous-time multi-armed bandit problem where decision opportunities arrive at Poisson arrival times, and study its Gittins index policy. When driven by spectrally one-sided Lévy processes, the Gittins index can be written explicitly in terms of the scale function, and is shown to converge to that in the classical Lévy bandit of Kaspi and Mandelbaum (1995).

### [02144] Optimal Consumption with Loss Aversion and Reference to Past Spending Maximum

**Format :** Talk at Waseda University

**Author(s) :** Xun LI (The Hong Kong Polytechnic University) Xiang Yu (The Hong Kong Polytechnic University) Zhang Qinyi (The Hong Kong Polytechnic University)

**Abstract :** This talk studies an optimal consumption problem for a loss-averse agent with reference to past consumption maximum. To account for loss aversion on relative consumption, an S-shaped utility is adopted that measures the difference between the non-negative consumption rate and a fraction of the historical spending peak. We consider the concave envelope of the realization utility with respect to consumption, allowing us to focus on an auxiliary HJB variational in- equality on the strength of concavification principle and dynamic programming arguments. By applying the dual transform and smooth-fit conditions, the auxiliary HJB variational inequality is solved in closed-form piecewisely and some thresholds of the wealth variable are obtained. The optimal consumption and investment control of the original problem can be derived analytically in the piecewise feedback form. The rigorous verification proofs on optimality and concavification principle are provided. Some numerical sensitivity analysis and financial implications are also presented.

### [02873] On the Entropy martingale optimal transport

**Format :** Talk at Waseda University

**Author(s) :** Shuoqing Deng (The Hong Kong University of Science and Technology) Erhan Bayraktar (University of Michigan) Dominykas Norgilas (University of Michigan)

**Abstract :** We study the Entropy Martingale Optimal Transport of Doldi and Frittelli (Finance&Stochastics, 2023). Compared with classical MOT, marginal constraints and linear pricing rules are respectively replaced by penalisation on deviations from the reference measures and utility-induced nonlinear rules. Inspired by techniques from classical MOT, we prove the duality with different arguments and weaker conditions. In particular, combining minimax arguments and the optional decomposition theorem, we generalise their duality without continuity requirement for the dynamic strategy.

### [02785] Functional convex order for the McKean-Vlasov equation

**Format :** Talk at Waseda University

**Author(s) :** Yating Liu (Paris Dauphine University) Gilles Pagès (Sorbonne University)

**Abstract :** We introduce the functional convex order for two McKean-Vlasov processes  $X$  and  $Y$  with respective marginal distributions  $(\mu_t)_{t \in \mathbb{N}}$

**[0, T]}** and  $\{\nu_t\}_{t \in [0, T]}$

**[0, T]}.** For a convex functional  $G$

defined on the product space involving the path space and its marginal distribution space, we obtain  $\mathbb{E}G(X, \{\mu_t\}_{t \in [0, T]}) \leq \mathbb{E}G(Y, \{\nu_t\}_{t \in [0, T]})$  under appropriate conditions. This presentation also includes two applications of the convex order result to mean-field control and mean-field games.

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00382 (2/3) : 2D @D514 [Chair: Xiaolu Tan]

### **[03167] Incentive to shape equilibria in double auction markets**

**Format :** Talk at Waseda University

**Author(s) :** Thibaut Mastrolia (UC Berkeley) Mathieu Rosenbaum (Ecole Polytechnique) Joffrey Derchu (Ecole Polytechnique)

**Abstract :** We study a toy two-player game for periodic double auction markets with imperfect information between the players. It allows us to link market spreads with signal strength. We first derive some market statistics related to the model studied. Then, we characterize Nash equilibria in cases with or without incentives from the exchange. This enables us to derive new insights about price formation and incentives design.

### **[04566] On time-consistent equilibrium stopping under aggregation of diverse discount rates**

**Format :** Talk at Waseda University

**Author(s) :** Jiacheng Zhang (UC Berkeley) Shuoqing Deng (The Hong Kong University of Science and Technology) Xiang Yu (The Hong Kong Polytechnic University)

**Abstract :** This paper studies the central planner's decision making on behalf of a group of members with diverse discount rates. In the context of optimal stopping, we work with a smooth aggregation preference to incorporate all heterogeneous discount rates with an attitude function that reflects the aggregation rule in the same spirit of ambiguity aversion in the smooth ambiguity preference proposed in Klibanoff et al. (2005). The optimal stopping problem renders to be time inconsistent, for which we develop an iterative approach using consistent planning and characterize all time-consistent equilibria as fixed points of an operator in the setting of one-dimensional diffusion processes. We provide some sufficient conditions on both the underlying models and the attitude function such that the smallest equilibrium attains the optimal equilibrium in which the attitude function becomes equivalent to the linear aggregation rule as of diversity neutral. When the sufficient condition of the attitude function is violated, we can illustrate by various examples that the characterization of the optimal equilibrium may differ significantly from some existing results for an individual agent, which now sensitively depends on the attitude function and the diversity distribution of discount rates.

### **[02775] CONVERGENCE OF POLICY IMPROVEMENT FOR ENTROPY-REGULARIZED STOCHASTIC CONTROL PROBLEMS**

**Format :** Talk at Waseda University

**Author(s) :** Yu-Jui Huang (University of Colorado, Boulder) Zhenhua Wang (University of Michigan) Zhou Zhou (University of Sydney)

**Abstract :** For a general entropy-regularized stochastic control problem on an infinite horizon, we prove that a policy improvement algorithm (PIA) converges to an optimal relaxed control. Contrary to the standard stochastic control literature, classical Hölder estimates of value functions do not ensure the convergence of the PIA, due to the added entropy-regularizing term. To circumvent this, we carry out a delicate estimation by moving back and forth between appropriate Hölder and Sobolev spaces. This requires new Sobolev estimates designed specifically for the purpose of policy improvement and a nontrivial technique to contain the entropy growth. Ultimately, we obtain a uniform Hölder bound for the sequence of value functions generated by the PIA, thereby achieving the desired convergence result. Characterization of the optimal value function as the unique solution to an exploratory Hamilton–Jacobi–Bellman equation comes as a by-product.

## [03347] Continuous time q-learning for McKean-Vlasov control problems

**Format :** Talk at Waseda University

**Author(s) :** Xiaoli Wei (Tsinghua Shenzhen International Graduate School) Xiang Yu (The Hong Kong Polytechnic University)

**Abstract :** For continuous time McKean-Vlasov control problems, we study the continuous time version of Q-learning for reinforcement learning under entropy regularization. Due to the complexity of distribution dependence, the counterpart of the martingale characterization of q-function in the single-agent control problem fails in our framework. To resolve the challenge, we introduce two distinct q-functions, which share the same integral under all test stochastic policies. The first q-function is associated to the optimal policy and policy improvement, and the second q-function can be used to develop the weak martingale characterization of some related processes under all test stochastic policies. Based on the weak martingale characterization and the relationship between two q-functions, we can design some q-learning algorithms for the learning McKean-Vlasov control problems and present several financial applications.

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00382 (3/3) : 2E @D514 [Chair: Kazutoshi Yamazaki]

## [02892] Skew Brownian Motion with Two-Valued Drift

**Format :** Talk at Waseda University

**Author(s) :** Xiaowen Zhou (Concordia University)

**Abstract :**

We consider a skew Brownian motion with two-valued drift as the unique solution to the following SDE  
 $dX_t = (\mu_- I_{\{X_t \leq a\}} + \mu_+ I_{\{X_t > a\}})dt + dB_t + \beta dL^a_t(X)$ ,  
where  $\mu_-$  and  $\mu_+$  are constants,  $-1 < \beta < 1$ ,  $B$  is a Brownian motion and  $L^a_t(X)$  denotes the symmetric local time for  $X$  at level  $a$ . Such a process can be identified as a regime switching model depending on whether the process  $X$  takes values above or below level  $a$ . In this talk we present some properties for such processes and discuss an optimization problem that is motivated by the optimal dividend problem for risk processes.

This talk is based on joint work with Zhongjin Gao.

## [02928] Pathwise uniqueness of SDEs driven by stable processes

**Format :** Talk at Waseda University

**Author(s) :** Hiroshi Tsukada (Kagoshima University)

**Abstract :** We consider one-dimensional stochastic differential equations (SDEs) driven by strictly stable processes. In this talk, we give some non-Lipschitz conditions on diffusion and drift coefficients under which the pathwise uniqueness of solutions to the SDEs is established. Moreover, we provide sufficient conditions for the non-contact property of strong solutions to the SDEs with different initial values.

## [05583] Mean field portfolio games

**Format :** Talk at Waseda University

**Author(s) :** Guanxing Fu (The Hong Kong Polytechnic University)

**Abstract :** We study mean field portfolio games, which is proved to be equivalent to an (F)BSDE, by martingale optimality principle and dynamic programming principle. A key implication is the uniqueness result of the game. Closed form solution is possible under stronger assumptions. If time permits, I will introduce possible extensions.

## [03375] A mean-field version of Bank--El Karoui's representation of stochastic processes

**Format :** Talk at Waseda University

**Author(s) :** Xiaolu Tan (The Chinese University of Hong Kong)

**Abstract :** We investigate a mean-field version of Bank--El Karoui's representation theorem of stochastic processes. Under different technical conditions, we established some existence and uniqueness results. As motivation and first applications, the results of mean-field representation provide a unified approach for studying various mean-field games (MFGs) in the setting with common noise and multiple populations, including the MFG of timing and the MFG with singular control, etc. As a crucial technical step, a stability result was provided on the classical Bank--El Karoui's representation theorem. It has its own interests and other applications, such as deriving the stability results of optimizers (in the strong sense) for a class of optimal stopping and singular control problems.

# [00384] Origami Engineering (1/2)

**Session Time & Room :**

00384 (1/3) : 2D (Aug.22, 15:30-17:10) @F411

00384 (2/3) : 2E (Aug.22, 17:40-19:20) @F411

00384 (3/3) : 3C (Aug.23, 13:20-15:00) @F411

**Type :** Proposal of Minisymposium

**Abstract :** Discussions on topics related to origami engineering will take place at this mini-symposium. Presenters will present their research aimed at applying the technology of origami, the folding of flat materials to create shapes, to engineering, and exploring the geometric properties of origami from a mathematical perspective to explore its range of applications.

**Organizer(s) :** Jun Mitani, Sachiko Ishida, Kazuya Saito

**Classification :** 51-08, 74A05, 70B10, 74K25, 74S05, Origami

**Minisymposium Program :**


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00384 (1/3) : 2D @F411 [Chair: Jun Mitani]

## [01360] Farthest point map on the double cover of a parallelotope

**Format :** Talk at Waseda University

**Author(s) :** Yoshikazu Yamagishi (Ryukoku University)Sayaka Ueda (Ryukoku University)

**Abstract :** We describe the source unfolding on the double cover of a parallel polytope of dimension n. Suppose two persons p,q play the squash in a parallelotope. Where is the farthest point q from a given point p? What happens if they keep playing the squash by choosing the farthest points? It is shown that the limit set is a union of quadratic curves.

## [01518] Deployable earwig fan dome with the algorithmic design tool

**Format :** Talk at Waseda University

**Author(s) :** Chisaki KITAJIMA (Kyushu University)Kazuya Saito (Kyushu University)

**Abstract :** Earwigs can fold their wing most compactly of all insects, therefore the characteristics have potential for engineering applications. In previous studies, we have already revealed how to design the crease pattern of the earwigs fan. Here we show a method to create three-dimensional forms from the folding simulation of the earwig fan with an algorithmic design tool. Furthermore, we propose to design compactly foldable dome-shape structures based on crease pattern of earwig fan.

## [01519] Geometry and mechanics of molting in snakes and caterpillars

**Format :** Talk at Waseda University

**Author(s) :** Taiju Yoneda (Kyushu University)Kazuya Saito ( Kyushu University)

**Abstract :** Snakes and caterpillars have longer bodies and grow by molting, but the molting process is different.

Snakes molt by reversing the front and back of their skin. In the molting of caterpillars, their skin is folded with buckling.

Which mode is expected to be determined by geometric factors such as thickness and mechanical factors such as friction. We quantify these boundary conditions using a combination of buckling experiments and finite element method with cylindrical shell models.

## [01523] Linear transformation of crease pattern boundaries preserving internal graph isomorphisms

**Format :** Talk at Waseda University

**Author(s) :** Yohei Yamamoto (University of Tsukuba)

Jun Mitani (University of Tsukuba)

**Abstract :** A crease pattern whose boundaries are similar before and after flat-folding can be tiled to create larger origami works. In order to increase the variation, linearly transforming the boundary shape is a useful approach, but if the entire crease pattern is transformed, the flat-foldability is not maintained. We propose a method for linear transformation of the boundaries while preserving internal graph isomorphisms. The characteristics of generated crease patterns and the folded states are discussed.

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00384 (2/3) : 2E @F411 [Chair: Yoshikazu Yamagishi]

## [01571] Laboratory-scale Workshop for Enhancing Designability of Origami Cores

**Format :** Talk at Waseda University

**Author(s) :** Sachiko Ishida (Meiji University)

**Abstract :** The objective of this study is to develop a laboratory-scale fabrication method to prototype origami-like foldable cores with our own designs. As the first attempt, we formed honeycomb cores in such a way that thermoplastic sheets were pressed between heated molds with corrugated configuration and glued together. This method worked well to enhance designability of honeycomb cores, because the press forming was applicable even for complex designs and could improve shape accuracy.

## [01618] Strip folding as Boolean matrix algebra and its Categorical Meanings

**Format :** Talk at Waseda University

**Author(s) :** Yiyang Jia (Seikei University)Jun Mitani (University of Tsukuba)

**Abstract :** Strip folding, known as map folding in the one-dimensional case, derives from a classical flat-foldability decision problem in the field of computational origami. In this manuscript, different from the existing computational and algorithmic methodology, we investigate strip folding using abstract algebraic language and then characterize it from a categorical viewpoint. We first present a boolean matrix description of strip folding, based on which we then build the category of strip folding. This category gives rise to a natural meet semi-lattice structure. Furthermore, in this category, every product exists. We use the right adjoint functor of the diagonal functor to define these products. Furthermore, the definition of products can be used to build a Grothendieck topology in the space of flatly folded states. Our result shows that the analysis of strip folding can be associated with contemporary mathematical methodologies such as category theory and algebraic geometry.

## [02328] Application of the proposed method to a transport origami box

**Format :** Online Talk on Zoom

**Author(s) :** Toshie Sasaki (Meiji University)Yang Yang (Meiji University)Ichiro Hagiwara (Meiji University)

**Abstract :** Fruits and vegetables are damaged during transportation because there is a mortal frequency band for each transport. We propose a new method named “Energy Density Topology Changing Method” based on the fact that the eigen frequency is determined by equivalent stiffness and equivalent mass. We demonstrate the effectiveness of this method by showing that it can be successfully applied to a transport origami box which cannot be applied by conventional topology optimization method.

00384 (3/3) : 3C @F411 [Chair: Tomohiro Tachi]

## [01536] Refoldability between polyhedra

**Format :** Talk at Waseda University

**Author(s) :** Tonan Kamata (Japan Advanced Institute of Science and Technology)

**Abstract :** Refolding is an operation of reshaping a polyhedron into a polyhedron by cutting open the surface of the original one and folding the resulting unfolding to make the other one. Refolding is a natural subject with applications in space engineering, design engineering, and bioinformatics, but the known result is not so much. In this talk, we will present design methods of refolding for some specific classes of polyhedra and the possibility of reconfiguration by refoldings.

## [05407] Optimal Simple Fold-and-Cut of a Polygonal Line

**Format :** Talk at Waseda University

**Author(s) :** Ryuhei Uehara (Japan Advanced Institute of Science and Technology)

**Abstract :** We investigate a natural variant of the fold-and-cut problem. We are given a long paper strip  $P$  and a polygonal line, which consists of a sequence of line segments, drawn on  $P$ . We cut all the line segments by one complete straight cut after overlapping all of them by a sequence of simple foldings. Our goal is to minimize the number of simple foldings to do that. When the polygonal line satisfies some certain geometric conditions, we can find a shortest sequence of simple foldings for the given polygonal line that consists of  $n$  line segments in  $O(n^3)$  time and  $O(n^2)$  space.

## [02335] Geometrical Comparison of Two kinds of Pairing Origami Polyhedron and Their Application to Beverage Containers

**Format :** Online Talk on Zoom

**Author(s) :** Aya Abe (Meiji University)Yang Yang (Meiji University)Chie Nara (Meiji University)Ichiro Hagiwara (Meiji University)

**Abstract :** Tachi-Miura Polyhedron is gaining attention as a 3-dimensional version of Miura-Ori. Meanwhile, Nojima Polyhedron is similar as TMP in that it can be folded both in the axial and radial direction. In this study, whether both are rigid folding or not is geometrically confirmed, and quantitatively considered how it affects the energy absorption properties. As a result, it effects the deformation modes but does not affect the purpose of investigating the feasibility of industrialization.

## [00385] Origami Engineering (2/2)

**Session Time & Room :**

00385 (1/2) : 3D (Aug.23, 15:30-17:10) @F411

00385 (2/2) : 3E (Aug.23, 17:40-19:20) @F411

**Type :** Proposal of Minisymposium

**Abstract :** Discussions on topics related to origami engineering will take place at this mini-symposium. Presenters will present their research aimed at applying the technology of origami, the folding of flat materials to create shapes, to engineering, and exploring the geometric properties of origami from a mathematical perspective to explore its range of applications.

**Organizer(s) :** Jun Mitani, Sachiko Ishida, Kazuya Saito

**Classification :** 51-08, 74A05, 70B10, 74K25, 74S05, Origami

**Minisymposium Program :**

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00385 (1/2) : 3D @F411 [Chair: Tonan Kamata]

## [01402] Solitons in Origami / Kirigami Tessellations and Their Underlying Dynamical Systems

**Format :** Talk at Waseda University

**Author(s) :** Rinki Imada (The University of Tokyo)Tomohiro Tachi (The University of Tokyo)

**Abstract :** The non-uniform folding of origami/kirigami tessellation, the folding where the configuration of their unit cell isn't identical, is potentially a great source of nonlinear phenomena. We can mathematically understand these phenomena by the nature of the dynamical systems induced by their geometry.

In this presentation, we report the “soliton-like” phenomenon with the propagation of localized deformation in origami/kirigami tessellations which comes from different mechanisms, i.e., the homoclinic/heteroclinic solutions of their dynamical systems.

## [01403] Macroscopic Behavior of Kirigami Tessellations with Contact Surfaces

**Format :** Talk at Waseda University

**Author(s) :** Akito Adachi (The University of Tokyo)Tomohiro Tachi (The University of Tokyo)

**Abstract :** Origami and kirigami tessellations with contact surfaces have potential applications including flexible electronics and wearable devices. However, the manufacturing process requires a simultaneous folding of all creases, which makes the pattern difficult to be manufactured. In this study, we reveal the macroscopic behavior of kirigami variations with contact surfaces through singular value decomposition of the kinematic deformation of each module; through this study, we explore the possibility of manufacturing such tessellations by tension-induced buckling.

## [01432] Miura fold bending in two directions and their combination

**Format :** Talk at Waseda University

**Author(s) :** Sora Moriyama (The University of Tokyo)Tomohiro Tachi (The University of Tokyo)Kuo-chih Chuang (Zhejiang University)

**Abstract :** For Miura folds, where the unit cell is usually composed of parallelograms, it is known that folds that are not parallel to the row's direction can be deformed in-plane after folding. If the unit cell is constructed so that it has different angles in the column's direction, it is deformable out-of-plane after folding. By understanding and combining these mathematically, we will present the Miura fold, which can be deformed in any direction.

## [01526] Development study of foldable and portable comfortable acoustic space

**Format :** Online Talk on Zoom

**Author(s) :** Keiko Yamazaki (Meiji University)Masanori Hashiguchi (KEISOKU ENGINEERING SYSTEM CO., LTD.)Daih Mi (KEISOKU ENGINEERING SYSTEM CO., LTD.)Ichiro Hagiwara (Meiji University)

**Abstract :** The purpose of our research is to develop a simple sound-reducing shade to enjoy playing music at home. The requirements for the shade are relatively inexpensive, foldable, suitable size and acoustic environment for playing, and most importantly sound dampening ability. Normally, the development of such a product requires many prototypes and verifications, but in this research, by utilizing finite element analysis to find the optimum material and shape without producing a large number of prototypes.

00385 (2/2) : 3E @F411 [Chair: Akito Adachi]

## [01562] A remark on the foldability of non-simply connected paper

**Format :** Talk at Waseda University

**Author(s) :** Hiroko Murai (Nara Women's University)Akari Iwamura (Nara Women's University)

**Abstract :** It is known that for any simply connected piece of paper  $P$ , any flat folded state  $(f, \lambda)$  of  $P$  is realized by a motion from the unfolded state.

In this talk, we show that the above result does not hold if the paper is not simply connected and give some examples.

## [05414] Origami Structures and Materials: Energy Absorption and Impact Mechanics

**Format :** Talk at Waseda University

**Author(s) :** Guoxing Lu (Swinburne University of Technology)

**Abstract :** This presentation introduces energy absorption and impact response of origami inspired structures and metamaterial, which we have recently studied. Several examples of incorporating the concepts of origami will be presented. They include thin-walled structures under axial loading, Miura metamaterials and its variations under quasi-static and dynamic compression and origami sandwich panels under quasi-static loading and ballistic impact.

Responses of such materials and structures involve large plastic deformation as well as dynamic effects. For metamaterials, analytical models have been developed to describe the strength and energy absorption capacity. It is assumed that the base material is ductile and can be approximated as a perfectly-plastic material. The analytical model is verified by the numerical simulations as well as quasi-static compression test of a four-sheet origami specimen. Response of such material under impact loading is also investigated and a shock model is proposed for high velocity impact.

## [02536] Platonic solids-based optimization for kirigami honeycomb fabrication of complex structures

**Author(s) :** Junichi Shinoda (Interlocus CO.LTD)Keiko Yamazaki (Meiji University)Ichiro Hagiwara (Meiji University)Luis Diago (Meiji University)

**Abstract :** The aerospace, automotive, and marine industries are heavily reliant on sandwich panels with cellular material cores. In this work, a platonic solids-based optimization algorithm has been developed to select the direction of the cells of the kirigami-honeycomb panel with the smallest waste of materials by rotating the 3D solid model of any shape according to the normal vectors in the platonic solids.

## [02542] Development of beautifully foldable PET bottles

**Author(s) :** Yang Yang (Meiji University)Chie Nara (Meiji University)Ichiro Hagiwara (Meiji University)

**Abstract :** Although many have attempted to develop a PET bottle that is foldable in the axial direction without bending, such bottles are not yet on the market. This is because that although the model with several foldable layers can be folded rather easily without bending, it springs back to almost its original height after compression. Thus, we develop new types of PET bottle with two or three spiral layers to resolve this spring back issue.

# [00389] Randomized methods for solving linear systems and eigenvalue problems

## Session Time & Room :

00389 (1/3) : 2C (Aug.22, 13:20-15:00) @E811

00389 (2/3) : 2D (Aug.22, 15:30-17:10) @E811

00389 (3/3) : 2E (Aug.22, 17:40-19:20) @E811

## Type : Proposal of Minisymposium

**Abstract :** Although the field of randomized numerical linear algebra has grown significantly, developments on accurate randomized solvers only start to emerge in recent years. This minisymposium intends to bring together researchers to exchange ideas on producing fast and accurate randomized solvers, studying their performance, and exploring new applications. We will specifically focus on randomized methods for solving linear systems and eigenvalue problems and on randomized strategies that can produce reliable high-quality solutions or approximations. Some topics include randomized iterative solvers, preconditioning, matrix approximations, low-rank compression, and eigenvalue detection. Applications to PDE solutions, machine learning, and data analysis will also be discussed.

**Organizer(s) :** Jianlin Xia, Qiang Ye

**Classification :** 68W20, 65F05, 65F08, 65F15, 65F55

## Minisymposium Program :

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00389 (1/3) : 2C @E811 [Chair: Qiang Ye]

## [03670] Making the Nyström method highly accurate for low-rank approximations

### Format : Online Talk on Zoom

**Author(s) :** Jianlin Xia (Purdue University)

**Abstract :** The Nyström method is a convenient method to quickly obtain a low-rank approximation to a kernel matrix with low or modest accuracies. In this work, we propose a type of Nyström methods that can reach high accuracies. The methods (called high-accuracy Nyström methods) treat the Nyström method and a skinny rank-revealing factorization as a fast pivoting strategy in a progressive alternating direction refinement process. A rank expansion strategy based on fast subset updates is further proposed and can quickly advance the sizes of the basis matrices. A fast randomized accuracy control strategy is also given. Different versions of high-accuracy Nyström methods are derived and can produce low-rank approximations with prespecified accuracies, sometimes with near SVD quality.

## [04016] Superfast iterative refinement of Low Rank Approximation of a Matrix

### Format : Online Talk on Zoom

**Author(s) :** Victor Pan (CUNY)

**Abstract :** Every superfast (aka sublinear cost) Low Rank Matrix Approximation (LRA) algorithm -- involving much fewer flops and memory cells than matrix has entries -- cannot work on ANY input, failing even with randomization, but our LRA algorithms are efficient or nearly optimal for MANY (large class of) inputs. Moreover, we propose, analyze, and test novel superfast algorithms for iterative refinement of any crude but sufficiently close LRA, according to both formal study and numerical tests.

## [00881] Relaxation in low-rank updates of Schur complement preconditioners in fluid flow problems

### Format : Talk at Waseda University

**Author(s) :** Sabine Le Borne (Hamburg University of Technology)

**Abstract :** In the simulation of fluid dynamic problems we often have to solve large-scale saddle-point systems. Low-rank updates can adapt standard preconditioners and accelerate convergence. We consider a low-rank correction for pressure Schur complement preconditioners and introduce a relaxation of the initial preconditioner which can improve the update scheme. Numerical results for the linearized Navier-Stokes equations illustrate the action of the update scheme.

## [00530] Randomized low-rank approximations beyond Gaussian random matrices

**Format :** Online Talk on Zoom

**Author(s) :** Arvind Krishna Saibaba (North Carolina State University)Agnieszka Miedlar (Virginia Tech)

**Abstract :** Randomized algorithms have been a revolutionary force in the field of low-rank approximations. A key step in these randomized algorithms is the randomized range finder which involves products with random matrices. The prevalent approach is to take the random matrix to be standard Gaussian which has favorable theoretical properties and is easy to implement in practice. Although several non-Gaussian random matrices have been used and analyzed, there are many open questions on what classes of random matrices are suitable for the randomized range finder. We analyze three different classes of random matrices: independent subgaussian entries, independent subgaussian columns, and independent bounded columns. These bounds provide a unified approach to studying various classes of random matrices and are supported by numerical experiments on test and real-world matrices.

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00389 (2/3) : 2D @E811 [Chair: Jianlin Xia]

## [04523] Are randomized NLA algorithms numerically stable?

**Format :** Talk at Waseda University

**Author(s) :** Yuji Nakatsukasa (University of Oxford)Joel A. Tropp (Caltech)

**Abstract :** We develop algorithms for linear systems and eigenvalue problems that apply fast randomized sketching to accelerate standard subspace projection methods, such as GMRES and Rayleigh-Ritz. This modification allows for incorporating nontraditional bases for the approximation subspace. When the basis is numerically full rank, these algorithms have accuracy similar to classic methods but run faster. We illustrate a 70x speedup over gmres. Time (and progress) permitting, I will discuss recent developments in related topics.

## [05547] Randomized orthogonalization process

**Format :** Online Talk on Zoom

**Author(s) :** Laura Grigori (EPFL and PSI)

**Abstract :** In this talk we will review recent progress on deriving algorithms for orthogonalizing a set of vectors. We will discuss then how this algorithms could be used to solve linear systems of equations and eigenvalue problems. We will conclude with numerical experiments that show the numerical stability of the proposed algorithms.

## [04952] A robust randomized indicator method for accurate symmetric eigenvalue detection

**Format :** Online Talk on Zoom

**Author(s) :** Zhongyuan Chen (Medical College of Wisconsin)Jiguang Sun (Michigan Technological University)Jianlin Xia (Purdue University)

**Abstract :** We propose a robust randomized indicator method for accurate eigenvalue detection for symmetric matrices  $A$ , which gives a novel way to use randomization to design eigensolvers for finding interior eigenvalues. An indicator detects the existence of eigenvalues inside an interval based on some statistical norm estimators for a spectral projector. Previous work on eigenvalue indicators relies on a threshold which is only heuristically chosen, thus often resulting in spurious or missed eigenvalues. In this work, we use rigorous statistical analysis to guide the design of a robust indicator. Multiple randomized estimators for a contour integral operator in terms of  $A$  are analyzed. In particular, when  $A$  has eigenvalues inside a given interval, we show that the failure probability (for the estimators to return very small estimates) is extremely low. This enables to design a robust rejection indicator based on the control of the failure probability. We then illustrate how the indicator method may potentially be used to develop new randomized symmetric eigensolvers, where fast indicator evaluation via shifted linear system solution is employed in a bisection scheme. Unlike previous indicator methods that only produce eigenvalues, our method can conveniently reuse computations from indicator evaluations to find eigenvectors with little extra cost.

## [05321] The Adversarially Robust Generalized Eigenvalue Problem

**Format :** Online Talk on Zoom

**Author(s) :** Ming Gu (UC Berkeley)Jiaming Wang (UC Berkeley)

**Abstract :** In this talk, we will introduce novel algorithms for solving the adversarially robust generalized eigenvalue problem, a highly non-convex optimization problem that has long eluded traditional optimization solvers. We will first discuss the rank-one case and then move on to the general-rank case. We will also show the potential applications of our algorithms in robust adaptive beamforming.

00389 (3/3) : 2E @E811 [Chair: Jianlin Xia]

## [03799] Stochastic Gradient Descent with Conjugate Gradient-style Momentum

**Format :** Online Talk on Zoom

**Author(s) :** Bao Wang (University of Utah)Qiang Ye (University of Kentucky)

**Abstract :** Momentum may be crucial in stochastic gradient-based optimization algorithms for convergence acceleration. The classical conjugate gradient algorithm may be considered as gradient descent with momentum. In this talk, we introduce a stochastic gradient descent algorithm with a conjugate gradient-style momentum. We will discuss its convergence properties and present some numerical examples to demonstrate its effectiveness.

## [01342] Robust randomized preconditioning for kernel ridge regression

**Format :** Talk at Waseda University

**Author(s) :** Mateo Diaz Diaz (Johns Hopkins University)Ethan Epperly (Caltech)Zachary Frangella (Stanford)Joel Tropp (Caltech)Robert Webber (California Institute of Technology)

**Abstract :** We advocate two randomized preconditioning approaches for applying kernel ridge regression (KRR) to a moderate or large number of data points ( $N \geq 10^4$ ). RPCholesky preconditioning is guaranteed to solve the exact KRR equations involving the  $N \times N$  kernel matrix in just  $\mathcal{O}(N^2)$  operations, assuming eigenvalue decay. KRILL preconditioning is guaranteed to solve the restricted KRR equations involving a  $N \times k$  kernel submatrix in just  $\mathcal{O}((N + k^2)k \log k)$  operations, with no assumptions on the kernel matrix or the regularization parameter. Experiments with dozens of data sets validate the effectiveness of RPCholesky and KRILL. Additionally, our theoretical analysis shows that RPCholesky and KRILL have stronger robustness properties compared to other commonly used preconditioners.

## [01305] Structured matrix recovery using randomized matrix-vector products

**Format :** Talk at Waseda University

**Author(s) :** Diana Halikias (Cornell University)Alex Townsend (Cornell University)

**Abstract :** Can one recover a matrix efficiently from only matrix-vector products? If so, how many are needed? We describe randomized algorithms of this type for various structured matrices. In particular, we recover an  $N \times N$  hierarchical matrix with rank- $k$  off-diagonal blocks using  $\mathcal{O}(k \log(N))$  matrix-vector products. While existing algorithms employ a recursive “peeling” procedure of elimination, we use recursive projection, which may be preferable when matrix-vector products are noisy, or for recovering the nearest hierarchical matrix.

# [00390] Recent Advances in Machine Learning Theory and Applications

**Session Time & Room :**

00390 (1/2) : 1C (Aug.21, 13:20-15:00) @E804

00390 (2/2) : 1D (Aug.21, 15:30-17:10) @E804

**Type :** Proposal of Minisymposium

**Abstract :** Successful applications of machine learning algorithms usually motivate theoretical studies of their computational and consistent properties. These theoretical studies help researchers and practitioners better understand the algorithms, identify appropriate application domains, and set up hyperparameters to achieve the best performance. On the other side, theoretical studies can also in turn motivate new algorithms by addressing the limitations of existing algorithms. This usually improves the performance in some specific scenarios or broaden the application domains of the existing algorithms. This minisymposium will collect talks on recent advances that address the interplay of mathematical foundations of machine learning and their applications.

**Organizer(s) :** Andreas Christmann, Han Feng, Qiang Wu

**Classification :** 68Q32, 68T09

**Minisymposium Program :**

00390 (1/2) : 1C @E804 [Chair: Qiang Wu]

## [03668] Learning through empirical gain maximization

**Format :** Online Talk on Zoom

**Author(s) :** Yunlong Feng (State University of New York at Albany)Qiang Wu (Middle Tennessee State University)

**Abstract :** In this presentation, we introduce a novel empirical gain maximization (EGM) framework for addressing robust regression problems with heavy-tailed noise or outliers in the response variable. EGM focuses on approximating the noise distribution's density function rather than directly approximating the truth function. This approach, stemming from minimum distance estimation, allows for the exclusion of abnormal observations, unlike traditional maximum likelihood estimation. We demonstrate that well-known robust nonconvex regression techniques, such as Tukey regression and truncated least square regression, can be reformulated within this new framework. By developing a learning theory for EGM, we provide a unified analysis for these established, yet not fully-understood, regression methods. This framework offers fresh insights into existing bounded nonconvex loss functions and reveals close connections between seemingly unrelated terminologies, such as Tukey's biweight loss and the triweight kernel. We also show that other prevalent bounded nonconvex loss functions in machine learning can be reinterpreted from specific smoothing kernels in statistics. Lastly, our framework facilitates the creation of new bounded nonconvex loss functions for robust learning.

## [01357] SKELETAL BASED IMAGE PROCESSING FOR CNN BASED IMAGE CLASSIFICATION

**Format :** Online Talk on Zoom

**Author(s) :** Cen Li (Middle Tenn State University)Tsega Tsahai (Middle Tenn State University)

**Abstract :** This work studies image processing techniques as a preprocessing step in image classification. Deep Learning based Human Pose Estimation was used to preprocess raw image to extract key posture information, and CNN was applied to learn the classification models for human postures. Two applications have been developed: (1) teaching a humanoid robot to play an interactive game of Simon Says, (2) a fall detection system for elderly residents in an assisted living facility.

## [01023] Total stability of kernel methods and localized learning

**Format :** Online Talk on Zoom

**Author(s) :** Andreas Christmann (University of Bayreuth)Hannes Koehler (University of Bayreuth)

**Abstract :** Regularized kernel-based methods typically depend on the underlying probability measure P and very few hyperparameters.

We investigate the influence of simultaneous slight perturbations of P, the hyperparameters, and the kernel on the resulting predictor.

Furthermore, kernel methods suffer from their super-linear computational requirements for big data.

Hence we extend our results to the context of localized learning.

The talk is based on Koehler and Christmann, JMLR, 23, 1-41, 2022.

00390 (2/2) : 1D @E804 [Chair: Qiang Wu]

## [01397] Learning Ability of Interpolating Convolutional Neural Networks

**Format :** Talk at Waseda University

**Author(s) :** Tian-Yi Zhou (Georgia Institute of Technology)Xiaoming Huo (Georgia Institute of Technology)

**Abstract :** It is frequently observed that overparameterized neural networks generalize well. Regarding such phenomena, existing theoretical work mainly devotes to linear settings or fully connected neural networks. This paper studies the learning ability of an important family of deep neural networks, deep convolutional neural networks (DCNNs), under underparameterized and overparameterized settings. We establish the best learning rates of underparameterized DCNNs without parameter restrictions presented in the literature. We also show that, by adding well-defined layers to an underparameterized DCNN, we can obtain some interpolating DCNNs that maintain the good learning rates of the underparameterized DCNN. This result is achieved by a novel network deepening scheme designed for DCNNs. Our work provides theoretical verification of how overfitted DCNNs generalize well.

## [03542] Classification with Deep Neural Networks

**Format :** Talk at Waseda University

**Author(s) :** Lei Shi (Fudan University)Zihan Zhang (Fudan University & City University of Hong Kong)Dingxuan Zhou (University of Sydney)

**Abstract :** Classification with deep neural networks (DNNs) has made impressive advancements in various learning tasks. Due to the unboundedness of the target function, generalization analysis for DNN classifiers with logistic loss remains scarce. This talk will report our recent progress in establishing a unified framework of generalization analysis

for both bounded and unbounded target functions. Our analysis is based on a novel oracle-type inequality, which enables us to deal with the boundedness restriction of the target function. In particular, for logistic classifiers trained by deep fully connected neural networks, we obtain the optimal convergence rates only by requiring the Hölder smoothness of the conditional probability. Under certain circumstances, such as when decision boundaries are smooth and the two classes are separable, the derived convergence rates can be independent of the input dimension. This talk is based on joint work with Zihan Zhang and Prof. Ding-Xuan Zhou.

### [03729] Robust Deep Learning with Applications

**Format :** Talk at Waseda University

**Author(s) :** Qiang Wu (Middle Tennessee State University)Shu Liu (Middle Tennessee State University)

**Abstract :** Deep neural networks are playing increasing roles in machine learning and artificial intelligence. Their performance highly depends on the network architecture and the loss function. The classical square loss is widely known to be sensitive to outliers. We propose the use of robust loss and two stage algorithms for deep neural networks, which are able to extract robust features and deal with outliers effectively. Applications in regression analysis and adversarial machine learning will be discussed.

## [00391] Recent Advances in Multiscale Transforms for Image Analysis

**Session Time & Room :** 4D (Aug.24, 15:30-17:10) @A502

**Type :** Proposal of Minisymposium

**Abstract :** This minisymposium will bring together researchers working on multiscale image transforms beyond wavelets and discuss deeper connections between harmonic analysis and image analysis. We plan to discuss various methods to decompose an image into "predictable" local segments and their residuals that allow efficient and sparse image approximation and associated tools based on new types of directional wavelets and monogenic signal representations. The key idea here is how to predict main features, e.g., dominant orientation information in texture images, in each local segment in such a way that the unpredictable portion in that segment is easily compressible or remains as noise.

**Organizer(s) :** Naoki Saito, Katsu Yamatani

**Classification :** 94A08, 42C40, 42C10, 62H25, 62H11

**Minisymposium Program :**

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00391 (1/1) : 4D @A502 [Chair: Naoki Saito/Katsu Yamatani]

### [01735] Multiscale monogenic image representations using Poisson kernels

**Format :** Talk at Waseda University

**Author(s) :** Brian Knight (University of California, Davis)Naoki Saito (University of California, Davis)

**Abstract :** By viewing a 1D signal as the boundary value of a harmonic function in the unit disc in  $\mathbb{C}$ , one can obtain a multiscale analytic signal representation by supplementing its conjugate counterpart. This is done by the Poisson/Cauchy integral formula. We generalize this for a 2D image by sandwiching it by quaternionic Poisson/Cauchy kernels. This leads to a natural multiscale monogenic image representation. We also plan to discuss its application in oriented texture image analysis.

### [02090] Image Interpolation Technique by the PCA of the Gradient Distribution

**Format :** Talk at Waseda University

**Author(s) :** Masaki Morita (Meijo University)Yuto Kimura (Meijo University)Katsu Yamatani (Meijo University)Masayoshi Nakagawa (Meijo University)

**Abstract :** We propose a method to reconstruct local image patches with gradient data and boundary information. In this talk, we present an image interpolation technique based on the principal component analysis of the gradient distribution of image intensities. Our numerical experiments show superiority of our proposed method over previous method based on the interpolation using harmonic functions.

## [02079] Improvement of coding procedures for Haar transform-based lossy image compression

**Format :** Talk at Waseda University

**Author(s) :** Keita Ashizawa (Shizuoka Institute of Science and Technology)Katsu Yamatani (Meijo University)

**Abstract :** We discuss an improved version of our Multi–neighbor Predictors and Residual Orthogonal Transformations, MPROT, which was a Haar transform-based lossy image compression method without generating mosquito noise. Due to the slow decay of the Haar coefficients, however, the PSNR values of certain test images compressed by the MPROT were not entirely satisfactory. Our new coding scheme takes advantage of redundancy of the MPROT coefficients and improves high-resolution image compression quality.

## [02086] Edge enhancement with directional wavelet transform

**Format :** Talk at Waseda University

**Author(s) :** Kensuke Fujinoki (Kanagawa University)Keita Ashizawa (National Institute of Technology, Maizuru College)

**Abstract :** We introduce a two-dimensional directional discrete wavelet transform that can decompose an image into twelve multiscale nearly isotropic directional edge components. The transform is designed in fully discrete setting and therefore is easy to implement in the spatial domain. Experimental results for image edge detection and enhancement show that both global and local edge structures of images are successfully represented.

# [00400] Bilevel optimization in machine learning and imaging sciences

**Session Time & Room :**

00400 (1/2) : 2C (Aug.22, 13:20-15:00) @A618

00400 (2/2) : 2D (Aug.22, 15:30-17:10) @A618

**Type :** Proposal of Minisymposium

**Abstract :** In the framework of functional minimisation approaches, the task of customising the functional expression of both the prior and the likelihood terms to the data at hand by means of a further optimisation problem has been recently popularised under the name of bilevel optimisation. In this minisymposium, we gather experts working in such field both from theoretical and algorithmic perspectives with the intent of providing an overview of how bilevel learning can be effectively employed to estimate data-adaptive regularisation and data models for both imaging and machine learning applications.

**Organizer(s) :** Luca Calatroni, Samuel Vaienti

**Classification :** 46N10, 65K10, 90C26

**Minisymposium Program :**

00400 (1/2) : 2C @A618 [Chair: Luca Calatroni/Samuel Vaienti]

## [03653] Fixed-Point Automatic Differentiation of Forward--Backward Splitting Algorithms for Partly Smooth Functions

**Format :** Talk at Waseda University

**Author(s) :** Sheheryar Mehmood (University of Tuebingen)Peter Ochs (Saarland University)

**Abstract :** A large class of non-smooth practical optimization problems can be written as minimization of a sum of smooth and partly smooth functions. We consider such structured problems which also depend on a parameter vector and study the problem of differentiating its solution mapping with respect to the parameter which has far reaching applications in sensitivity analysis and parameter learning optimization problems. We show that under partial smoothness and other mild assumptions, Automatic Differentiation (AD) of the sequence generated by proximal splitting algorithms converges to the derivative of the solution mapping. For a variant of automatic differentiation, which we call Fixed-Point Automatic Differentiation (FPAD), we remedy the memory overhead problem of the Reverse Mode AD and moreover provide faster convergence theoretically. We numerically illustrate the convergence and convergence rates of AD and FPAD on Lasso and Group Lasso problems and demonstrate the working of FPAD on prototypical practical image denoising problem by learning the regularization term.

## [05289] A framework for bilevel optimization that enables stochastic and global variance reduction algorithms

**Format :** Talk at Waseda University

**Author(s) :** Thomas Moreau (Inria - MIND)

**Abstract :** Bilevel optimization, the problem of minimizing a value function that involves the arg-minimum of another function, appears in many areas of machine learning. In a large-scale empirical risk minimization setting where the number of samples is huge, it is crucial to develop stochastic methods, which only use a few samples at a time to progress. However, computing the gradient of the value function involves solving a linear system, which makes it difficult to derive unbiased stochastic estimates. To overcome this problem we introduce a novel framework, in which the solution of the inner problem, the solution of the linear system, and the main variable evolve at the same time. These directions are written as a sum, making it straightforward to derive unbiased estimates. The simplicity of our approach allows us to develop global variance reduction algorithms, where the dynamics of all variables are subject to variance reduction. This allows to design near-optimal algorithms to solve the bi-level problem.

## [03309] Bilevel Optimization with a Lower-level Contraction: Optimal Sample Complexity without Warm-Start

**Format :** Talk at Waseda University

**Author(s) :** Saverio Salzo (Sapienza Università di Roma)Riccardo Grazzi (Istituto Italiano di Tecnologia)Massimiliano Pontil (Istituto Italiano di Tecnologia)

**Abstract :** We present a stochastic algorithm for a general class of bilevel problems consisting of a minimization problem at the upper-level and a fixed-point equation at the lower-level. This setting includes instances of meta-learning, equilibrium models, and hyperparameter optimization. The main feature of our solution is to avoid using the warm-start procedure at the lower-level, which is not always well-suited in applications, and yet to achieve order-wise optimal or near-optimal sample complexity.

## [02768] Bilevel subspace optimisation in heterogeneous clustering for cryo-EM

**Format :** Talk at Waseda University

**Author(s) :** Willem Diepeveen (University of Cambridge)Carlos Esteve-Yagüe (University of Cambridge)Jan Lellmann (University of Lübeck)Ozan Öktem (KTH Royal Institute of Technology)Carola-Bibiane Schönlieb (University of Cambridge)

**Abstract :** In heterogeneous Cryo-EM we are concerned with retrieving protein conformations from noisy 2D projection images. Attempting to solve this directly is challenging in the absence of a good prior. In recent work, it has been observed that MD simulations live on low-dimensional manifold of conformation space. Although this subspace might not be a perfect reflection of reality, it potentially yields a good prior. In this work we attempt to use this information in Cryo-EM conformation retrieval. In particular, we aim to retrieve conformations and the actual manifold from Cryo-EM data, but we want the manifold to match the MD data. We propose a bilevel optimisation approach to this problem.

00400 (2/2) : 2D @A618 [Chair: Luca Calatroni/Samuel Vaiter]

## [05645] Test like you train in implicit deep learning

**Author(s) :** Pierre Albin (Apple)

**Abstract :** Implicit deep learning relies on expressing some components of deep learning pipelines implicitly via a root equation. The training of such a model is thus a bi-level optimization. In practice, the root equation is solved using a fixed number of iterations of a solver. We discuss the effect of having a different number of iterations at test time than at train time, challenging a popular assumption that more iterations at test time improve performance.

## [00404] Large-Scale Eigenvalue Computations and Optimization

**Session Time & Room :**

00404 (1/2) : 1C (Aug.21, 13:20-15:00) @E603

00404 (2/2) : 1D (Aug.21, 15:30-17:10) @E603

**Type :** Proposal of Minisymposium

**Abstract :** The minisymposium aims at presenting a few recent developments in large-scale eigenvalue computations and optimization, as well as investigating the intimate connection between them. Of particular interest are not only standard and generalized eigenvalue problems but also nonlinear eigenvalue problems, multiparameter eigenvalue problems, singular value decompositions, and their applications such as those in data science and control theory. Orthogonal transformations and projections to proper subspaces play vital roles for computing and optimizing eigenvalues numerically in the large-scale setting. The minisymposium focuses on the use of such tools in modern algorithms for large-scale eigenvalue computations, optimization, and applications.

**Organizer(s) :** Kensuke Aishima, Emre Mengi

**Classification :** 65F15

**Minisymposium Program :**

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00404 (1/2) : 1C @E603 [Chair: Kensuke Aishima]

### [03074] Consistent Estimation Using SVD for a Linear Regression Model

**Format :** Talk at Waseda University

**Author(s) :** Kensuke Aishima (Hosei University)

**Abstract :** In this talk, we consider parameter estimation of an errors-in-variables linear regression model. The standard approach to such parameter estimation is to formulate an optimization problem and solve it numerically using the singular value decomposition (SVD). Using the property that the SVD identifies the image and null spaces of a matrix, with orthogonal projections to the subspaces, we derive a consistent estimator for a linear regression model with the errors in a subset of variables.

### [04078] Fast optimization of eigenvalues for frequency-based damping of second-order systems

**Format :** Online Talk on Zoom

**Author(s) :** Nevena Jakovčević Stor (University of Split)Tim Mitchell (Queens College / CUNY)Zoran Tomljanović (University of Osijek)Matea Ugrica (Max Planck Institute for Dynamics of Complex Technical Systems)

**Abstract :** We consider optimizing eigenvalues of certain parametric second-order systems that model vibrating mechanical systems, where the goal is to achieve frequency-weighted damping by moving eigenvalues away from undesirable areas on the imaginary axis. We present two new complementary approaches for this task. First, we propose determining damper viscosities via solving new nonsmooth constrained optimization problems. Second, we also propose a fast new eigensolver for the structured quadratic eigenvalue problems that appear in such vibrating systems.

### [02304] Rectangular multiparameter eigenvalue problems

**Format :** Talk at Waseda University

**Author(s) :** Bor Plestenjak (University of Ljubljana)Michiel E Hochstenbach (TU Eindhoven)Tomaž Košir (University of Ljubljana)

**Abstract :** In a rectangular multiparameter eigenvalue problem we have a  $k$ -variate,  $k \geq 2$ , polynomial pencil of rectangular matrices  $W(\lambda) \in \mathbb{C}^{(n+k-1) \times n}$  and  $\lambda_0 \in \mathbb{C}^k$  is an eigenvalue if  $\text{rank}(W(\lambda_0))$

### [04501] Simultaneous diagonalization and new bounds on shared invariant subspaces

**Format :** Talk at Waseda University

**Author(s) :** Brian Sutton (Randolph-Macon College)

**Abstract :** Commuting Hermitian matrices may be simultaneously diagonalized by a common eigenvector matrix. However, the numerical aspects are delicate, and existing Jacobi-like algorithms have a prohibitively large operation count on large matrices. We derive new error bounds on shared invariant subspaces and use them to develop a new simultaneous diagonalization algorithm with a running time that is a small multiple of a single eigenvalue-eigenvector computation.

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00404 (2/2) : 1D @E603 [Chair: Emre Mengi]

### [03188] Estimation of the dominant poles of a large-scale descriptor system

**Format :** Talk at Waseda University

**Author(s) :** Emre Mengi (Koc University)

**Abstract :** The dominant poles of the transfer function of a descriptor system are those poles that can cause large frequency response. They can be used to form reduced-order approximations to the system. We describe a subspace

framework to estimate the dominant poles of a large-scale descriptor system based on Petrov-Galerkin projections. The projection subspaces are expanded gradually by means of the dominant poles of the projected systems. We argue formally that the framework converges quadratically.

### [03212] Subspace Methods for Nonlinear Eigenvalue Problems

**Format :** Talk at Waseda University

**Author(s) :** Rifqi Aziz (Koc University)Emre Mengi (Koc University)Matthias Voigt (UniDistance Suisse)

**Abstract :** We will discuss numerical methods for nonlinear eigenvalue problems that are described by matrices of large dimension. We project the large matrices within an interpolatory framework in order to obtain a reduced nonlinear eigenvalue problem that can be solved more efficiently. Based on the eigenpair residuals, new interpolation points and corresponding projection matrices can be computed in order to obtain a few eigenvalues close to a desired target point.

### [05296] Optimizing orthogonality in large-scale tensor networks

**Format :** Talk at Waseda University

**Author(s) :** Roel Van Beeumen (Lawrence Berkeley National Laboratory)

**Abstract :** Orthogonality plays a key role in eigenvalue computations. In 1D tensor networks such as tensor trains, the orthogonality is maintained by using QR or truncated SVD factorizations. However, this technique does not extend to 2D tensor networks such as projected entangled pair states (PEPS). Moreover, orthogonality inside a PEPS keeps the computational complexity of eigenvalue evaluations bounded. We will discuss and compare several approximate orthogonalization techniques and strategies for orthogonalizing PEPS columns and rows.

### [05462] Linearizability of eigenvector nonlinearities

**Format :** Online Talk on Zoom

**Author(s) :** Elias Jarlebring (KTH Royal Institute of Technology)

**Abstract :** We present a method to linearize, without approximation, a specific class of eigenvalue problems with eigenvector nonlinearities (NEPv), where the nonlinearities are expressed by scalar functions that are defined by a quotient of linear functions of the eigenvector. The exact linearization relies on an equivalent multiparameter problem (MEP) that contains the exact solutions of the NEPv. Based on the linearization we propose numerical schemes that exploit the structure of the linearization.

## [00410] Recent advances in Bayesian optimal experimental design

**Session Time & Room :** 2D (Aug.22, 15:30-17:10) @G304

**Type :** Proposal of Minisymposium

**Abstract :** Computational measurement models may involve several uncertain parameters in addition to the unknown quantities of primary interest. In Bayesian optimal experimental design, the goal is to design a measurement configuration, e.g. optimal placement of sensors to collect observational data, which maximizes the expected utility---such as the expected information gain---for obtaining information on the unknown quantities subject to uncertainties in the measurement model. This is especially important when there is a limited budget for collecting actual measurement data. This minisymposium showcases recent theoretical and computational developments to overcome the major challenges encountered in problems arising within this field.

**Organizer(s) :** Claudia Schillings, Vesa Kaarnioja

**Classification :** 65Cxx, 62Kxx, 62Fxx

**Minisymposium Program :**

00410 (1/1) : 2D @G304 [Chair: VESA KAARNIOJA]

### [04376] A transport map approach for Bayesian optimal experimental design

**Format :** Talk at Waseda University

**Author(s) :** Karina Koval (Heidelberg University)Roland Herzog (Heidelberg University)Robert Scheichl (Heidelberg University)

**Abstract :** Solving the Bayesian optimal experimental design (BOED) problem requires optimizing an expectation of a utility function or optimality criterion that assesses the quality of each design. For Bayesian inverse problems with non-Gaussian posteriors, a closed-form expression for the criterion is typically unavailable. Thus, access to a computationally efficient approximation is crucial for numerical solution of the optimal design problem. We propose a flexible approach

for approximating the expected utility function and solving the BOED problem that is based on transportation of measures. The key to our method is the approximation of the joint density on the design, observation and inference parameter random variables via the pushforward of a simple reference density under an inverse Knothe-Rosenblatt (KR) rearrangement. This KR map exposes certain conditional densities which enables approximation of the optimality criterion for any design choice. We present our approach and assess the effectiveness of the resulting optimal designs with some numerical examples.

## [04957] Accelerating A-Optimal Design of Experiments Using Neural Networks

**Format :** Talk at Waseda University

**Author(s) :** Jinwoo 4702324183 Go (Georgia Institute of Technology)Peng Chen (Georgia Institute of Technology)

**Abstract :** Designing experiments for large-scale problems demands significant computational resources, and Partial Differential Equation (PDE) surrogates have emerged as a widely-adopted approach to address this challenge. This study enhances this methodology by independently training PDE surrogates and their Jacobians. Leveraging the trained Jacobian of PDEs, we approximate the posterior covariance matrix. Subsequently, we compute the trace of this matrix and evaluate the reduction in uncertainty resulting from executing the experimental setup.

## [05059] Stability of Bayesian optimal experimental design in inverse problem

**Format :** Talk at Waseda University

**Author(s) :** Tapiro Helin (LUT University)Jose Rodrigo Rojo Garcia (LUT University)Duc-Lam Duong (LUT University)

**Abstract :** In this talk, I will explore the stability properties of Bayesian optimal experimental design towards misspecification of distributions or numerical approximations. Specifically, I will present a framework for addressing this problem in a non-parametric setting, and demonstrate a stability result for the expected utility with respect to likelihood perturbations. To provide a more concrete illustration, I will then consider non-linear Bayesian inverse problems with Gaussian likelihood, where the forward mapping is replaced by an approximation.

## [05080] Quasi-Monte Carlo methods for Design of Experiment

**Format :** Talk at Waseda University

**Author(s) :** Claudia Schillings (FU Berlin)Vesa Kaarnioja (Free University of Berlin)FU Berlin

**Abstract :** Bayesian experimental design aims to optimize the placement of measurements in an experiment such that information about unknown quantities is maximized (w.r. to a suitable criterion). The optimization problem requires the evaluation of the information gain, which corresponds to the evaluation of an integral w.r. to the posterior distribution. We will explore the use of quasi-Monte Carlo methods for Bayesian design problems in this talk and present convergence results.

# [00413] Numerical Methods for Dispersive PDEs and Applications

**Session Time & Room :**

00413 (1/2) : 4D (Aug.24, 15:30-17:10) @G605

00413 (2/2) : 4E (Aug.24, 17:40-19:20) @G605

**Type :** Proposal of Minisymposium

**Abstract :** Dispersive partial differential equations (PDEs) play a fundamental role in many fields such as the nonlinear optics, water wave theory, quantum mechanics, etc. From the perspective of computational mathematics, it is significant to design efficient numerical methods to solve dispersive PDEs with in-depth numerical analysis and provide an intuitive view for physical phenomena. The proposed minisymposium invites experts in this field to review recent advances in numerical methods for dispersive PDEs and applications.

**Organizer(s) :** Weizhu Bao, Yue Feng

**Classification :** 35Q41, 65M15, 65M70

**Minisymposium Program :**

00413 (1/2) : 4D @G605 [Chair: Weizhu Bao]

## [05510] Numerical studies of two regularized versions of the cubic NLS

**Format :** Online Talk on Zoom

**Author(s) :** Christof Sparber (University of Illinois Chicago)

**Abstract :** We consider two types of regularization for the focusing, cubic nonlinear Schrödinger equation (NLS) posed in two and/or three spatial dimensions. One type of regularization is given by a defocusing quintic nonlinearity, while the other is given by a second order elliptic differential operator, describing off-axis variations of the NLS in the context of laser physics. While the non-regularized NLS is known to exhibit finite-time blow-up, these augmented equations are proved to be globally well-posed. In both cases we numerically investigate the long time behavior of solutions using a time-splitting method. In particular, we are interested in the orbital (in-)stability of least action ground states in the radially symmetric case. This is joint work with Christian Klein, Rémi Carles, and Jack Arbunich.

## [05557] Dirac equations for the modeling of electron dynamics on strained graphene surfaces

**Format :** Talk at Waseda University

**Author(s) :** Emmanuel Lorin de la Grandmaison (Carleton University)

**Abstract :** This talk is devoted to the modelling of the dynamics of electrons on strained graphene surfaces. A hierarchy of mathematical models will be derived, and some numerical experiments illustrating the scattering of wave packets on locally deformed graphene will be proposed

## [02732] Low regularity exponential-type integrators for the "good" Boussinesq equation

**Format :** Talk at Waseda University

**Author(s) :** Chunmei Su (Tsinghua University) Hang Li (Tsinghua University )

**Abstract :** We introduce a series of semi-discrete low regularity exponential-type time integrators for the "good" Boussinesq equation. Compared to the existing numerical methods, the temporal convergence of ours can be achieved under weaker regularity assumptions on the exact solutions. The methods are constructed based on twisted variables and some harmonic analysis techniques in approximating the exponential integral. The methods are explicit and easy to be implemented efficiently when combined with pseudospectral method for spatial discretization.

## [04017] Computational methods for stationary states of nonlinear Schrödinger/Gross-Pitaevskii equations

**Format :** Talk at Waseda University

**Author(s) :** Wei Liu (National University of Singapore)

**Abstract :** I will present some recent advances in the computation of stationary-state solutions to the nonlinear Schrödinger/Gross-Pitaevskii equations, primarily in the context of Bose-Einstein condensation. The (normalized) energy ground/excited states and action ground states will be mainly considered. Based on the analysis of variational characterizations and stabilities/instabilities for these stationary-state solutions, efficient and accurate numerical methods utilizing novel artificial dynamical flows and/or optimization techniques will be developed, with further extensions to challenging high-spin or fast-rotating models.

00413 (2/2) : 4E @G605 [Chair: Yue Feng]

## [05499] Scattering and uniform in time error estimates for splitting method in NLS

**Format :** Online Talk on Zoom

**Author(s) :** Rémi Carles (CNRS & Univ Rennes) Chunmei Su (Tsinghua University)

**Abstract :** We consider the nonlinear Schrödinger equation with a defocusing nonlinearity which is mass-(super)critical and energy-subcritical. We prove uniform in time error estimates for the Lie-Trotter time splitting discretization. This uniformity in time is obtained thanks to a vectorfield which provides time decay estimates for the exact and numerical solutions. This vectorfield is classical in scattering theory and requires several technical modifications compared to previous error estimates for splitting methods.

## [05587] Resonances as a computational tool

**Format :** Online Talk on Zoom

**Author(s) :** Katharina Schratz (Sorbonne University)

**Abstract :** A large toolbox of numerical schemes for dispersive equations has been established, based on different discretization techniques such as discretizing the variation-of-constants formula (e.g., exponential integrators) or splitting the full equation into a series of simpler subproblems (e.g., splitting methods). In many situations these classical schemes allow a precise and efficient approximation. This, however, drastically changes whenever non-smooth phenomena enter the scene such as for problems at low regularity and high oscillations. Classical schemes fail to capture the oscillatory nature of the solution, and this may lead to severe instabilities and loss of convergence. In this talk I present a new class of resonance based schemes. The key idea in the construction of the new schemes is to tackle and deeply embed the underlying nonlinear structure of resonances into the numerical discretization. As in the continuous case, these terms are central to structure preservation and offer the new schemes strong geometric properties at low regularity.

## [01752] Error estimates of numerical methods for the nonlinear Schrödinger equation with low regularity potential and nonlinearity

**Format :** Talk at Waseda University

**Author(s) :** Weizhu Bao (National University of Singapore) Chushan Wang (National University of Singapore)

**Abstract :** We prove optimal error bounds of time-splitting methods and the exponential wave integrator for the nonlinear Schrödinger equation ( $\text{NLSE}$ ) with low regularity potential and nonlinearity, including purely bounded potential and locally Lipschitz nonlinearity. Arising from different physical applications, low regularity potential and nonlinearity are introduced into the NLSE such as the discontinuous potential or non-integer power nonlinearity, which make the error estimates of classical numerical methods very subtle and challenging.

## [00418] Nonlinear PDE: beyond the well-posedness theory

**Session Time & Room :** 2C (Aug.22, 13:20-15:00) @F402

**Type :** Proposal of Minisymposium

**Abstract :** The theory of nonlinear partial differential equations (PDEs) is of fundamental importance in mathematical analysis, and through recent developments, it has reached a stage where some difficult and important questions beyond the well-posedness theory can be fruitfully addressed. The aim of this session focuses on a large class of nonlinear PDEs particularly related to Hamilton-Jacobi equations, level-set mean curvature flow equations, mean field games, and reaction diffusion equations, and brings experts to give a constructive and inspiring reflection on the state of the literature surrounding such equations, which will boost some further research in related areas.

**Organizer(s) :** Hiroyoshi Mitake, Hung Vinh Tran

**Classification :** 49L25, 53E10, 35Q89, 35K57

**Minisymposium Program :**

00418 (1/1) : 2C @F402 [Chair: Hiroyoshi Mitake, Hung V. Tran ]

## [01572] Hessian Riemannian flows in mean-field games

**Format :** Talk at Waseda University

**Author(s) :** Diogo Gomes (KAUST)

**Abstract :** Hessian Riemannian flows are a powerful tool for the construction of numerical schemes for monotone mean-field games that have their origin in constrained optimization problems. In this talk, we discuss the general construction of these flows for monotone mean-field games, their existence and regularity properties, and their asymptotic convergence.

## [02413] Homogenization of Reactions in Random Media

**Format :** Talk at Waseda University

**Author(s) :** Yuming Paul Zhang (Auburn University) Andrej Zlatoš (University of California, San Diego)

**Abstract :** Homogenization is a general phenomenon when physical processes in periodic or random environments exhibit homogeneous long time dynamic due to large space averaging of the variations in the environment. While this area of Mathematics saw a slew of remarkable developments in the last 20 years, the progress in the case of reaction-diffusion equations has been somewhat limited due to the homogenized dynamic involving discontinuous solutions to part\_1

different (first-order) equations. In this talk I will discuss stochastic homogenization for reaction-diffusion equations in several spatial dimensions. These include the cases of both time-independent and time-dependent reactions, with the later proof employing a new subadditive ergodic theorem for time-dependent environments. This talk is based on joint works with Andrej Zlatoš.

### [02535] Continuum limit of dislocations with annihilation in one dimension

**Format :** Talk at Waseda University

**Author(s) :** Norbert Pozar (Kanazawa University)

**Abstract :** In this talk I discuss the many-particle limit for a system of particles in one dimension. The particles carry a signed charge, interact via a Newtonian potential and when two particles with opposite charges meet, they annihilate and are removed from the system. This serves as a simplified model of dislocation dynamics in a crystalline lattice. This talk is based on joint work with Mark Peletier and Patrick van Meurs.

### [04586] Quantitative periodic homogenization of a front propagation model in dynamic environments

**Format :** Talk at Waseda University

**Author(s) :** Wenjia Jing (Tsinghua University)

**Abstract :** In this talk we review the developments of homogenization theory for a front propagation model. It is described by a first order Hamilton-Jacobi equation with a Hamiltonian that grows linearly with respect to the absolute value of the momentum variable. We focus on the case of dynamic environment where the Hamiltonian has highly oscillations in time as well as in space. We present some key steps in the proof of the qualitative homogenization theory and in the quantification of the convergence rate in the periodic setting. The talk is based on several joint works with Souganidis, Tran and Yu.

## [00420] Painlevé equations, Applications, and Related Topics

**Session Time & Room :**

00420 (1/4) : 2D (Aug.22, 15:30-17:10) @A617

00420 (2/4) : 2E (Aug.22, 17:40-19:20) @A617

00420 (3/4) : 3C (Aug.23, 13:20-15:00) @A617

00420 (4/4) : 3D (Aug.23, 15:30-17:10) @A617

**Type :** Proposal of Minisymposium

**Abstract :** Recently, problems arising in statistical and probabilistic models with an underlying integrable structure have been found to possess deep links to continuous and discrete Painlevé equations.

The theory of Painlevé equations has therefore come to play an increasingly important role in the study of such problems. The way in which Painlevé equations appear, and the types of equations that appear in these problems pose deep questions on the side of the theory of Painlevé equations.

This mini-symposium aims to bring together experts both in Painlevé equations and the broad range of problems in which they appear, and illustrate this interplay.

**Organizer(s) :** Anton Dzhamay, Alexander Stokes, Tomoyuki Takenawa, Ralph Willox

**Classification :** 34M55, 34M56, 14E07, 33C45, 37K20

**Minisymposium Program :**

00420 (1/4) : 2D @A617 [Chair: Ralph Willox]

### [04296] The Identification Problem for Discrete Painlevé Equations

**Format :** Talk at Waseda University

**Author(s) :** Anton Dzhamay (University of Northern Colorado and BIMSA)

**Abstract :** We describe a refined version of the discrete Painlevé equations identification problem. We emphasize that, in addition to determining the surface type of the equation, it is important to determine the actual translation element, up to conjugation, and to keep in mind possible special point configurations that can affect the symmetry group of the

equation. We illustrate this by a variety of examples that appear in applications, especially in the theory of orthogonal polynomials.

## [04597] Orthogonal polynomials and discrete Painlevé equations on the $D_5^{(1)}$ Sakai surface

**Format :** Talk at Waseda University

**Author(s) :** Alexander Stokes (The University of Tokyo)Anton Dzhamay (University of Northern Colorado)Galina Filipuk (University of Warsaw)

**Abstract :** We show that two recurrences coming from the theory of orthogonal polynomials are transformable to discrete Painlevé equations, which share the same surface type  $D_5^{(1)}$  in the Sakai classification scheme but are non-equivalent.

The surfaces associated with these recurrences do not have the full parameter freedom for their type, and we find the symmetry groups of these examples as subgroups of the extended affine Weyl group of type  $A_3^{(1)}$  from the generic case.

## [03019] Orthogonal polynomials, Schur flow and Painlevé equations

**Format :** Talk at Waseda University

**Author(s) :** Walter Van Assche (KU Leuven)

**Abstract :** We give a brief introduction to orthogonal polynomials on the unit circle and show how an exponential modification of the weight function leads to the Ablowitz-Ladik lattice equations for the recurrence coefficients (Verblunsky coefficients) of these polynomials. As shown by Periwal and Shevitz (1990) these orthogonal polynomials appear in unitary matrix models. The Verblunsky coefficients satisfy the discrete Painlevé II equation and the ratio of these coefficients satisfy Painlevé III. The Lax pair can be written in terms of the CMV matrix, which is a pentadiagonal infinite matrix similar to the Jacobi matrix for orthogonal polynomials on the real line.

## [04527] Symmetries of discrete Nahm systems and Normalizers in Coxeter groups

**Format :** Online Talk on Zoom

**Author(s) :** yang shi (Flinders university)Giorgio Gubbiotti (Università degli Studi di Milano)

**Abstract :** It is known that discrete Nahm systems arise as autonomous versions of Sakai's classification of discrete Painlevé equations. Here we study the groups of symmetries of these systems using the theory of normalizers of Coxeter groups developed by Brink and Howlett (Invent. Math., 1999).

00420 (2/4) : 2E @A617 [Chair: Tomoyuki Takenawa]

## [04366] On the bilinear equations of the Painlevé transcedents

**Format :** Talk at Waseda University

**Author(s) :** Hidetaka Sakai (University of Tokyo)Tatsuya Hosoi (University of Tokyo)

**Abstract :** The sixth Painlevé equation is a basic equation with three fixed singular points, corresponding to Gauss's hypergeometric differential equation among linear equations. Similar to hypergeometric equation, for nonlinear equations, we would like to determine the equation from the local behavior around the three singularities. In this talk, the sixth Painlevé equation is derived by imposing the condition that it is of type (H) at each three singular points for quadratic 4th-order differential equation.

## [04932] Large-degree asymptotics of Generalized Hastings-McLeod functions

**Format :** Talk at Waseda University

**Author(s) :** Robert Buckingham (University of Cincinnati)

**Abstract :** The Generalized Hastings-McLeod functions form an infinite sequence of solutions to the inhomogeneous Painlevé-II equation. The functions have recently arisen in a variety of random matrix and interacting particle system problems. Using Riemann-Hilbert analysis and the nonlinear steepest-descent method, we establish the leading-order asymptotic behavior inside and outside the pole region as the inhomogeneous term tends to infinity. This is joint work with Kurt Schmidt.

## [04515] Spaces of initial values for equations with the quasi-Painlevé property

**Format :** Online Talk on Zoom

**Author(s) :** Thomas Kecker (University of Portsmouth)

**Abstract :** Considering differential equations and Hamiltonian systems with the property that all movable singularities of all their solutions in the complex plane are algebraic poles (quasi-Painlevé property), we generalise the concept of the

Okamoto's space of initial values for these types of equations. Starting from a general equation with analytic coefficient functions, the construction of this space yields certain differential conditions on these functions that are equivalent to the resonances found e.g. by the (quasi-)Painlevé test.

## [02754] On the (quasi-)Painleve equations

**Format :** Online Talk on Zoom

**Author(s) :** Galina Filipuk (University of Warsaw)

**Abstract :** Painleve equations are second order nonlinear differential equations solutions of which have no movable critical points. They appear in many applications. For solutions of quasi-Painleve equations algebraic singularities are allowed. The so-called geometric approach may help in many cases to understand the nature of singularities. In this talk I shall present some recent results on the geometric approach for the Painleve and quasi-Painleve equations. This is a joint work with A. Stokes.

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00420 (3/4) : 3C @A617 [Chair: Anton Dzhamay]

## [03574] A dynamical systems approach to map enumeration

**Format :** Online Talk on Zoom

**Author(s) :** Joceline Lega (University of Arizona)

**Abstract :** Freud orbits are trajectories of discrete Painlevé equations that describe the evolution of recurrence coefficients for orthogonal polynomials. We will introduce a nonlinear transformation, which converts a Freud orbit into a solution that converges towards a fixed point along a center manifold. Subsequent analysis will lead to an asymptotic expansion whose terms are generating functions for map enumeration. Examples of map counts will be provided. This is joint work with Nick Ercolani and Brandon Tippings.

## [03010] An affine Weyl group action on the basic hypergeometric series

**Format :** Talk at Waseda University

**Author(s) :** Takao Suzuki (Kindai University)

**Abstract :** Recently, we formulated a higher order generalization of the  $q$ -difference Painlevé equations called the  $q$ -Garnier system in a framework of an extended affine Weyl group of type  $A_{2n+1}^{(1)} \times A_1^{(1)} \times A_1^{(1)}$ . On the other hand, the  $q$ -Garnier system admits a particular solution in terms of the basic hypergeometric series  ${}_n\phi_n$ . In this talk, we investigate an action of the extended affine Weyl group on  ${}_n\phi_n$ .

## [03311] On the growth properties of some families of birational maps

**Format :** Online Talk on Zoom

**Author(s) :** Giorgio Gubbiotti (Universita degli Studi di Milano) Michele Graffeo (Politecnico di Milano)

**Abstract :** We characterise the growth and integrability properties of a family of elements in the Cremona group of a complex projective space in dimension three using techniques from algebraic geometry. This collection consists of maps obtained by composing the standard Cremona transformation  $c_3 \in \text{Bir}(\mathbb{P}^3)$  with projectivities permuting the fixed points of  $c_3$  and the points over which  $c_3$  performs a divisorial contraction. Time permitting, we discuss the possible extensions of this construction to higher dimensions.

## [05042] Laguerre (q-Laguerre) Weight Recurrence and Geometric Theory of Painlevé equations

**Format :** Online Talk on Zoom

**Author(s) :** Jie Hu (Jinzhong University (晋中学院))

**Abstract :** The Sakai geometric theory of Painlevé equations is useful for identify difference or differential equations as corresponding Painlevé equations. In this talk we consider two examples of recurrence relations appearing in study of recurrence coefficients of semi-classical orthogonal polynomials, namely, polynomials with Laguerre weight and with the deformed q-Laguerre weight. Using the geometry, we give explicit change of variables matching these equations with some standard discrete Painlevé equations.

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00420 (4/4) : 3D @A617 [Chair: Alexander Stokes]

## [04054] Folding transformations for q-Painleve equations

**Format :** Online Talk on Zoom

**Author(s) :** Mikhail Bershtein (Kavli IPMU, Landau Institute and Skoltech)

**Abstract :** Folding transformation of the Painleve equations is an algebraic (of degree greater than 1) transformation between solutions of different equations. In 2005 Tsuda, Okamoto and Sakai classified folding transformations of differential Painleve equations. These transformations are in correspondence with automorphisms of affine Dynkin diagrams. We give a complete classification of folding transformations of the q-difference Painleve equations, these transformations are in correspondence with certain subdiagrams of the affine Dynkin diagrams (possibly with automorphism). The method is based on Sakai's approach to Painleve equations through rational surfaces.

Based on joint work with A. Shchechkin [arXiv:2110.15320]

## [04739] Laguerre (q-Laguerre) Weight Recurrence and Geometric Theory of Painlevé equations

**Format :** Online Talk on Zoom

**Author(s) :** Jie HU (Jinzhong University)

**Abstract :** Sakai's geometric theory of Painlevé equations is used to identify difference or differential equations with corresponding Painlevé equations. In this talk we will consider two classes of examples of recurrence coefficients of semi-classical orthogonal polynomials: Laguerre weight and the deformed  $q$ -Laguerre weight. We will give the identification procedure on how to deduce related solutions of canonical discrete Painlevé equations from coefficients. Meanwhile, we also give the explicit birational function of variables achieving that reduction.

## [00421] When random comes to the rescue of numerical computation

**Session Time & Room :** 4D (Aug.24, 15:30-17:10) @E506

**Type :** Proposal of Minisymposium

**Abstract :** The need of efficient IA and deep learning applications has impulse a new way of performing floating-point computations based on low precision representation formats and their corresponding hardware support.

Among the peculiarity raised is the need of operators, analyses, methodologies, and tools to estimate accuracy needs, overcome unwanted behaviors such as stagnation (numerical loss during sequences of tiny updates) and optimize performance.

In this minisymposium, we will focus on a few aspects of randomization in numerical computation, covering its advantages for IA applications, probabilistic error analysis, variant of stochastic rounding mode and the detection of numerical abnormalities and precision analysis.

**Organizer(s) :** David DEFOUR

**Classification :** 65CXX, 65YXX

**Minisymposium Program :**

00421 (1/1) : 4D @E506 [Chair: David DEFOUR]

## [02748] The computer arithmetic new deal: AI is pushing the frontier

**Format :** Talk at Waseda University

**Author(s) :** Eric Petit (Intel)

**Abstract :** Recent years have seen a tremendous number of new research contributions to computer arithmetic, challenging lower precision arithmetic and rounding mode, leaving the IEEE754 standard far behind. This all comes from the rise of AI workloads as one of the main driver in the data center software and architecture design. Keeping on par with the incredibly fast changing usage of computer arithmetic has push our algorithms, tools, and capacity to their limit.

This is an opportunity to rethink and redesign our approach about floating point hardware and software, promoting new tools and methodologies, and allowing ground breaking solution to be promoted to main stream software and hardware implementation.

In this talk I will provide some more context about this change and discuss some of the exciting work I am sharing with collaborators inside and outside intel.

## [01590] New stochastic rounding modes for numerical verification

**Format :** Talk at Waseda University

**Author(s) :** Bruno LATHUILIERE (EDF R&D)Nestor Demeure (Data and analytics services group, National Energy Research Scientific Computing Center, Berkeley)

**Abstract :** In the context of industrial code verification, the use of stochastic rounding modes allows to estimate the numerical quality of the results through multiple independent executions of the software. But in some rare cases, the introduction of stochastic rounding can lead to a runtime error because the software implicitly relies on the determinism of IEEE floating-point operations.

To overcome this problem, we propose new deterministic stochastic rounding modes: these maintain the stochastic properties between different executions of the software while guaranteeing the determinism of the floating operations having the same parameters within one execution. Results based on an implementation of the method in the Verrou tool will be presented.

## [04711] Stochastic rounding as a model of round-to-nearest

**Format :** Talk at Waseda University

**Author(s) :** Devan Sohier (LI-PaRAD, UVSQ)

**Abstract :** Round-to-nearest (RN), the default rounding mode in the omnipresent IEEE754 standard, is difficult to analyze. Deterministic bounds, as well as their refinements like interval arithmetic, generally prove overly pessimistic, compared to the day-to-day observations of numerical scientists. Stochastic rounding (SR) may be used as a model of RN, the results of which are easier to analyze, and closer to these observations. In this talk, I will present a methodology to analyze results of a SR simulation of RN. The widely used formula for the number of significant bits –  $\log \frac{\sigma}{\mu}$  can be refined and given a precise statistical ground in the case when the error has a normal distribution; when no normality assumption is substantiated, other tools based on Bernoulli estimations need to be used. Using SR as a model for RN also has some limits: SR does not present stagnation phenomena typical of RN, and SR also does not give the same results when the program recomputes twice the same operation. Finally, I will discuss flaws of various severeness of some software implementations of SR, and present some remarks regarding possible future implementations of SR, both in software and hardware.

## [03452] VPREC to analyze the precision appetites and numerical abnormalities of several proxy applications

**Format :** Talk at Waseda University

**Author(s) :** Roman Iakymchuk (Umeå University)Pablo de Oliveira Castro (Université Paris-Saclay)

**Abstract :** The energy consumption constraint for large-scale computing encourages scientists to revise the architecture design of hardware but also applications, algorithms, as well as the underlying working/ storage precision. We introduce an approach to address the issue of sustainable computations from the perspective of computer arithmetic tools. We employ the variable precision backend (VPREC) to identify parts of code that can benefit from smaller floating-point formats. Finally, we show preliminary results on several proxy applications.

## [00426] Variational methods for thin structures and free-boundary problems

**Session Time & Room :**

00426 (1/3) : 4C (Aug.24, 13:20-15:00) @F312

00426 (2/3) : 4D (Aug.24, 15:30-17:10) @F312

00426 (3/3) : 4E (Aug.24, 17:40-19:20) @F312

**Type :** Proposal of Minisymposium

**Abstract :** Thin structures are classically studied using variational methods and PDEs, and they may be described both by surfaces and by free interfaces. On one hand, surfaces appear for modeling soap films and biological membranes minimizing suitable energy functionals, like area and Canham-Helfrich functionals. On the other hand, free interfaces separate a domain whose boundary is free: it is not known a priori and it depends on the solution of a PDE. Such a free-boundary problems naturally arise in many different models in Physics and Engineering, like for instance the Bernoulli one-phase problem.

**Organizer(s) :** Giulia Bevilacqua, Luca Lussardi

**Classification :** 49J45, 49Q05, 49Q10, 35R35, 76D27

**Minisymposium Program :**

## [03469] On the Kircchoff-Plateau problem: critical points and regularity

**Format :** Talk at Waseda University

**Author(s) :** Giulia Bevilacqua (Università di Pisa)

**Abstract :** In this talk I will discuss some generalization of the Plateau problem, which in its classical form asks if it exists a surface of minimal area spanning a given boundary. First-order necessary conditions and regularity properties are studied when a thick rod (with non vanishing thickness) and/or an elastic curve are assigned as the boundary spanned by the surface.

## [02176] On Stationary Points of Polyconvex Functionals

**Format :** Talk at Waseda University

**Author(s) :** Riccardo Tione (MPI MiS Leipzig)Camillo De Lellis (Institute for Advanced Study)Guido De Philippis (Courant Institute of Mathematics)Antonio De Rosa (University of Maryland)Jonas Hirsch (Universität Leipzig)Bernd Kirchheim (Universität Leipzig)

**Abstract :** Quasi- and polyconvex energies arise naturally in modeling physical phenomena related to elasticity. From the mathematical viewpoint, a challenging question concerns the regularity of critical/stationary points and minimizers of these energies. My talk focuses on recent results in this direction concerning stationary points, i.e. critical points subject to outer and inner variations. I also address the application of this question to geometric measure theory.

## [04199] Minimization of the Canham-Helfrich within generalised Gauss graphs

**Format :** Talk at Waseda University

**Author(s) :** Anna Kubin (Politecnico di Torino)Luca Lussardi (Politecnico di Torino)Marco Morandotti (Politecnico di Torino)

**Abstract :** The Canham-Helfrich functional is the most widely used functional to study the equilibrium of biological membranes as a result of the competition between mean curvature and Gaussian curvature.

In this talk, we review some approaches to the minimisation problem for this functional and present novel results in the setting of generalised Gauss graphs.

This is joint work with Anna Kubin and Luca Lussardi.

## [03181] A capillarity theory approach to the analysis of soap films

**Format :** Online Talk on Zoom

**Author(s) :** Salvatore Stuvard (University of Milan)Darren King (New York University)Francesco Maggi (University of Texas at Austin)Antonello Scardicchio (Abdus Salam ICTP)

**Abstract :** I will present a variational model, based on Gauss' theory of capillarity, which describes soap films as sets of finite perimeter enclosing a prescribed volume of fluid and satisfying a spanning condition of homotopic type, rather than minimal surfaces. I will discuss the corresponding existence theory, the sharp regularity properties of the minimizers, their asymptotic behavior in the vanishing volume limit, and I will attempt a qualitative description of their local and global geometry.

## [04117] Stable Möbius bands obtained by isometrically deforming circular helicoids

**Format :** Talk at Waseda University

**Author(s) :** Eliot Fried (Okinawa Institute of Science and Technology)Vikash Chaurasia (Okinawa Institute of Science and Technology)

**Abstract :** We consider a variational problem for finding an isometric deformation from a (circular helicoid to a stable Möbius band. Helicoids with certain specific numbers of turns yield stable bands with  $(n=2k+1), (k \geq 1)$ , half twists and  $(n)$ -fold rotational symmetry. Each such band has the least energy of any stable competitor with the same number of half twists. Helicoids with other numbers of turns yield two stable bands with equal energy but different numbers of half twists.

## [02967] Rectifiability for flat singularities of higher codimension area minimizers

**Format :** Talk at Waseda University

**Author(s) :** Camillo De Lellis (Institute for Advanced Study)

Paul Minter (Princeton University)

Anna Skorobogatova (Princeton University)

**Abstract :** Integral currents provide a natural setting in which to study the Plateau problem, but permit the formation of singularities in area-minimizers. The problem of determining the size and structure of the interior singular set of an area-minimizer in this setting has been studied in great detail since the 1960s, with many ground-breaking contributions. When the codimension is higher than 1, due to the presence of singular points with high multiplicity flat tangent cones, little progress has been made since Almgren's celebrated  $(m-2)$ -Hausdorff dimension bound on the singular set, the proof of which has since been simplified by De Lellis and Spadaro.

In this talk I will discuss joint work with Camillo De Lellis and Paul Minter, in which we achieve  $(m-2)$ -rectifiability for the singular set.

## [03455] Interior regularity for stationary two-dimensional multivalued maps

**Format :** Talk at Waseda University

**Author(s) :** Jonas Hirsch (University of Leipzig) Luca Spolaor (UCSD)

**Abstract :**  $Q$ -valued maps minimizing a suitably defined Dirichlet energy were introduced by Almgren in his proof of the optimal regularity of area minimizing currents in any dimension and codimension. In this talk I will discuss the extension of Almgren's result to stationary  $Q$ -valued maps in dimension 2. This is joint work with Jonas Hirsch (Leipzig).

## [03306] Transport of currents and geometric Rademacher-type theorems

**Format :** Online Talk on Zoom

**Author(s) :** Paolo Bonicatto (University of Warwick)

**Abstract :** Given a vector field  $b$  on  $\mathbb{R}^d$ , one usually studies the transport/continuity equation drifted by  $b$  looking for solutions in the class of functions or at most in the class of measures. I will talk about recent efforts, motivated by the modeling of defects in crystalline materials, aimed at extending the previous theory to the case when the unknown is instead a family of  $k$ -currents in  $\mathbb{R}^d$ .

00426 (3/3) : 4E @F312 [Chair: Giulia Bevilacqua]

## [02741] Long time behavior and stability of surface diffusion flow

**Format :** Talk at Waseda University

**Author(s) :** Antonia Diana (Scuola Superiore Meridionale )

**Abstract :** We present a long-time existence and stability result for the surface diffusion flow in the flat torus.

According to this flow, smooth hypersurfaces move with the outer normal velocity given by the Laplacian of their mean curvature.

We show that if the initial set is sufficiently close'' to a stable critical set for the volume-constrained Area functional, then the flow exists for all times and asymptotically converges to a translation'' of the critical set.

## [03626] Graphical solutions to one-phase problems

**Format :** Talk at Waseda University

**Author(s) :** Hui Yu (National University of Singapore) Max Engelstein (University of Minnesota-Twin Cities) Xavier Fernandez-Real (Ecole Polytechnique Federale de Lausanne)

**Abstract :** The free boundaries of solutions (critical points of the functional) to the one-phase problem can have rich geometry. Such richness can be reduced by imposing the graphical condition.

In this talk, we show that if homogeneous minimizers are trivial in dimension  $k$ , then graphical solutions are trivial in dimension  $k+1$ . This works for both the classical one-phase problem as well as its thin counterpart.

This talk is based on a joint work with Max Engelstein (Minnesota) and Xavier Fernandez-Real (EPFL).

## [04656] Regularity of the optimal shapes for a class of integral functionals

**Format :** Online Talk on Zoom

**Author(s) :** Bozhidar Velichkov (Università di Pisa)

**Abstract :** This talk is dedicated to the regularity of solutions to the following variational problem

$$\min \left\{ J(\Omega) : \Omega \subset D \right\},$$

where  $D \subset \mathbb{R}^d$  is a given bounded open set and  $J$  is a functional of the form

$$J(\Omega) = \int_{\Omega} j(x, u_{\Omega}) dx + |\Omega|,$$

where  $j : D \times \mathbb{R} \rightarrow \mathbb{R}$  is a given "cost function" and  $u_{\Omega}$  is the solution to

$$-\Delta u_{\Omega} = f(x) \quad \text{in } \Omega, \quad u_{\Omega} \in H_0^1(\Omega),$$

where  $f : D \rightarrow \mathbb{R}$  is a fixed function. We will discuss the case  $j(x, u_{\Omega}) = -g(x)u_{\Omega}$ , which leads to a free boundary system of the form

\begin{align}

$$-\Delta u \Omega = f(x) & \quad \text{in } \Omega \\ -\Delta v \Omega = g(x) & \quad \text{in } \Omega \\ u \Omega = v \Omega = 0 & \quad \text{on } \partial \Omega \\ |\nabla u \Omega| |\nabla v \Omega| = 1 & \quad \text{on } \partial \Omega \end{align}$$

$$\end{align}$$

\end{align}

We will show that, if the functions  $f$  and  $g$  are positive and comparable, and if the dimension  $d$  of the ambient space is 2, 3, or 4, then any optimal set  $\Omega$  is  $C^{1,\alpha}$  smooth (and solves the above system in the classical sense). The talk is based on joint works with Giorgio Tortone (University of Pisa) and Francesco Paolo Maiale (Scuola Normale Superiore), and on a joint work with Giuseppe Buttazzo (University of Pisa), Francesco Paolo Maiale (Scuola Normale Superiore), Dario Mazzoleni (University of Pavia), and Giorgio Tortone (University of Pisa).

## [04579] Min-max minimal surfaces with contact angle conditions

**Format :** Online Talk on Zoom

**Author(s) :** Luigi De Masi (University of Padova)

**Abstract :** Existence and regularity of minimal surfaces (i.e. stationary points for area functional) has been an active topic of research for the last decades. When minimizing strategies produce just trivial solutions, min-max methods may be successfully used.

In this talk, based on a joint work with G. De Philippis, I will discuss min-max construction of a minimal surface  $\Sigma$  in a container  $\mathcal{M} \subset \mathbb{R}^3$  which meets  $\partial \mathcal{M}$  with a fixed angle.

# [00432] Empirically Driven Deep Learning Theory

**Session Time & Room :**

00432 (1/2) : 2D (Aug.22, 15:30-17:10) @E812

00432 (2/2) : 2E (Aug.22, 17:40-19:20) @E812

**Type :** Proposal of Minisymposium

**Abstract :** Deep learning has become increasingly popular recently due to its superior performance on a variety of tasks. However, understanding the mathematical foundations of deep networks is challenging because they are highly parameterized and built using complex computational heuristics.

This session features recent works in mathematical deep learning theory based on empirically-driven, phenomenological approaches: the works first reveal prevalent phenomena observed across multiple deep learning settings; then, they propose new mathematical explanations for these phenomena. These mathematical results give important insights into the generalization of deep nets, the efficiency of their optimization, and their robustness to adversarial noise and data imbalance.

**Organizer(s) :** X.Y. Han, Weijie Su

**Classification :** 68T07, 68T05, 93E35, 65D15, 90C26, Deep learning theory based on experimentally-discovered phenomena.

**Minisymposium Program :**

00432 (1/2) : 2D @E812 [Chair: X.Y Han & Weijie Su]

## [02983] How different optimizers select the global minimizer in deep learning

**Format :** Talk at Waseda University

**Author(s) :** Weinan E (Peking University)

**Abstract :** It has been observed in deep learning that different optimization process converges to different global minimum.

We analyze this process by studying the stability of the minimum for the optimization algorithm. We find numerically that in practice, the numerical solutions often live at the so-called "edge of stability". We also study the relationship between the "sharpness" and "non-uniformity" of the global minimum. We present arguments that confirm the hypothesis that flat solution tends to generalize better. This is joint work with Chao Ma of Stanford University and Lei Wu of Peking University.

## [03263] A Law of Data Separation in Deep Learning

**Format :** Talk at Waseda University

**Author(s) :** Hangfeng He (University of Rochester)Weijie Su (University of Pennsylvania)

**Abstract :** While deep learning has enabled significant advances in many areas of science, its black-box nature hinders architecture design for future artificial intelligence applications and interpretation for high-stakes decision makings. We addressed this issue by studying the fundamental question of how deep neural networks process data in the intermediate layers. Our finding is a simple and quantitative law that governs how deep neural networks separate data according to class membership throughout all layers for classification. This law shows that each layer improves data separation at a constant geometric rate, and its emergence is observed in a collection of network architectures and datasets during training. This law offers practical guidelines for designing architectures, improving model robustness and out-of-sample performance, as well as interpreting the predictions.

## [03057] Neural Collapse in Deep Learning

**Format :** Talk at Waseda University

**Author(s) :** Vardan Papyan (University of Toronto)

**Abstract :** In this talk, we'll delve into Neural Collapse - a recently discovered phenomenon in deep learning that emerges in the final phase of model training. Additionally, we'll explore how this phenomenon relates to the interpretability, robustness, and generalization performance of deep learning models.

## [03168] Memorization-Dilation: A Novel Model for Neural Collapse in Deep Neural Network Classifiers

**Format :** Online Talk on Zoom

**Author(s) :** Gitta Kutyniok (LMU Munich)Duc Anh Nguyen (---)Ron Levie (Technion)Julian Lienen (University of Paderborn)Eyke Hüllermeier (LMU Munich)

**Abstract :** The notion of neural collapse refers to several emergent phenomena that have been empirically observed across various canonical classification problems. In this talk, we introduce a more realistic mathematical model than the classical layer-peeled model, which takes both the positivity of the features and the limited expressivity of the network into account. For this, we then show results about the performance of the trained network in the sense of generalization properties.

00432 (2/2) : 2E @E812 [Chair: X.Y. Han & Weijie Su]

## [04878] Understanding Deep Learning Through Optimization Geometry

**Format :** Talk at Waseda University

**Author(s) :** Nathan Srebro (TTIC)

**Abstract :** I will survey the approach emerging in recent years for understanding deep learning through the optimization geometry in function space induced by the architecture. To appreciate this view, its ability to explain empirical phenomena, and also its limitations, we will see how many phenomena can be understood through a detailed study of optimization geometry in a simple deep linear model.

## [04289] Feature Learning in Two-Layer Neural Networks

**Format :** Talk at Waseda University

**Author(s) :** Murat Erdogdu (University of Toronto)

**Abstract :** We study the effect of gradient-based optimization on feature learning in two-layer neural networks. We consider the non-asymptotic setting, and we show that a network trained via SGD exhibits low-dimensional representations, with applications in learning a monotone single-index model.

## [03006] On the Implicit Geometry of Deep-net Classifiers

**Format :** Talk at Waseda University

**Author(s) :** Tina Behnia (University of British Columbia) Ganesh Ramachandra Kini (University of California, Santa Barbara) Vala Vakilian (University of British Columbia) Christos Thrampoulidis (University of British Columbia)

**Abstract :** The talk will address the following questions:

What are the unique structural properties of models learned by deep-net classifiers?

Is there an implicit bias towards solutions of a certain geometry and how does this vary across architectures and data?

Specifically, how does this implicit geometry change under label imbalances, and is it possible to use this information to design better loss functions for learning with imbalances?

## [05316] Does the loss function matter in overparameterized models?

**Format :** Online Talk on Zoom

**Author(s) :** Vidya Muthukumar (Georgia Institute of Technology)

**Abstract :** Recent years have seen substantial interest in a first-principles theoretical understanding of the behavior of overparameterized models that interpolate noisy training data, based on their surprising empirical success. In this talk, I compare classification and regression tasks in the overparameterized linear model. On the one hand, we show that with sufficient overparameterization, solutions obtained by training on the squared loss ( minimum-norm interpolation) typically used for regression, are identical to those produced by training on exponential and polynomially-tailed losses, typically used for classification. On the other hand, we show that there exist regimes where these solutions are consistent when evaluated by the 0-1 test loss function, but inconsistent if evaluated by the mean-squared-error test loss function. Our results demonstrate that: a) different loss functions at the training (optimization) phase can yield similar solutions, and b) a significantly higher level of effective overparameterization admits good generalization in classification tasks as compared to regression tasks.

## [00435] Multiscale Numerical Methods for Complex Fluids

**Session Time & Room :**

00435 (1/3) : 4C (Aug.24, 13:20-15:00) @D101

00435 (2/3) : 4D (Aug.24, 15:30-17:10) @D101

00435 (3/3) : 4E (Aug.24, 17:40-19:20) @D101

**Type :** Proposal of Minisymposium

**Abstract :** Focus of this mini-symposium will be on the modelling and computational aspects of multiscale coupling strategies and hybrid techniques -continuum, mesoscopic, atomistic- specifically applied to complex fluids, such as colloidal suspensions, granular media, polymeric systems and/or multiphase flows. The goal is, on one hand, to share state-of-the-art results on multiscale approaches in fluids, on the other to discuss technical issues on their computational modelling. We believe that this mini-symposium will foster new collaborations and contribute to further advances in the field.

**Organizer(s) :** Giulio Giusteri, Takashi Taniguchi, Marco Ellero

**Classification :** 76A05, 76A10, 76M28, 76M10, 76M12

**Minisymposium Program :**

00435 (1/3) : 4C @D101 [Chair: Takashi Taniguchi]

## [05277] Multi-Physics Simulations of Flow, Friction, and Reactions in Solid/Liquid Interface

**Format :** Talk at Waseda University

**Author(s) :** Momoji Kubo (Tohoku University)

**Abstract :** In recent years, due to strong demands for energy saving and carbon neutrality, maximizing energy utilization efficiency in automobiles, airplanes, etc. is required. Therefore, it is essential to establish the technologies for the super-low friction. In the present study, we employed our supercomputer "MASAMUNE-IMR" and successfully applied our large-scale molecular dynamics code "Laich" to clarifying the multi-physics processes of the flow, friction, and chemical reactions in the solid/liquid interfaces for realizing the super-low friction system.

## [02346] Numerical modeling of viscoelastic flows with high elasticity

**Format :** Talk at Waseda University

**Author(s) :** Laura Moreno (Universita degli Studi di Padova)Joan Baiges (Universitat Politecnica de Catalunya)Ramon Codina (Universitat Politecnica de Catalunya)

**Abstract :** Computing the viscoelastic fluid flow involves a wide range of difficulties, in particular when elasticity becomes dominant. These difficulties are considered one of the biggest challenges in computational rheology; this is known as the High Weissenberg Number Problem. This work presents different strategies to deal with the shortcomings that appear when the fluid is particularly elastic. These are carried out in the Finite Element framework and by using the Variational Multiscale formulation as a stabilization approach.

## [02354] DPD Simulation of Ultrasound Propagation through Liquid Water

**Format :** Talk at Waseda University

**Author(s) :** Petra Papež (National Institute of Chemistry, Ljubljana)Matej Praprotnik (National Institute of Chemistry, Ljubljana)

**Abstract :** We present a dissipative particle dynamics simulation of ultrasound propagation through liquid water. The effects of frequency and thermostat parameters are studied and discussed. We show that frequency and thermostat parameters affect not only the attenuation but also the computed speed of sound. The present study paves the way for development and optimization of a virtual ultrasound machine for large-scale biomolecular simulations.

## [04595] Machine-Learning for Accelerated Multi-Scale Polymer Flow Simulations

**Format :** Talk at Waseda University

**Author(s) :** John Jairo Molina (Kyoto University)Souta Miyamoto (Kyoto University)Yoshiki Ueno (Kyoto University)Takashi Taniguchi (Kyoto University)

**Abstract :** We develop a Bayesian Machine-Learning approach, based on a Gaussian Process Regression, to accelerate Multi-Scale Simulations (MSS) of polymer melt flows. In particular, we are able to learn the constitutive relation of entangled polymer melts (within the Doi-Takimoto model), which are then used within macroscopic flow solvers, drastically reducing the computational cost. We also show how ML can be used to reduce the statistical variance of a full MSS, significantly enhancing its computational efficiency.

00435 (2/3) : 4D @D101 [Chair: Giulio Giusteri]

## [03437] Simulation of micro-scale particulate motion in gases

**Format :** Talk at Waseda University

**Author(s) :** Duncan Lockerby (University of Warwick)Josiah Jordan (University of Warwick)

**Abstract :** Low-speed gas flow around micro-scale particles (e.g. soot and other pollutants), and through suspensions of particles, are rich in physics and challenging to simulate. The hydrodynamic reach of a single particle is broad, making application of conventional approaches (e.g. finite-volume CFD) computationally expensive. Furthermore, their scale renders the conventional Navier-Stokes equations, and associated boundary conditions, inaccurate. In this talk we discuss recent developments in simulating micro-scale particulate flows using the Method of Fundamental Solutions.

## [03686] Synchronized Molecular-Dynamics simulation of the thermal lubrication of an entangled polymer melt

**Format :** Talk at Waseda University

**Author(s) :** Shugo Yasuda (University of Hyogo)

**Abstract :** The thermo-rheological property of an entangled polymer melt in wall-driven shear flows is investigated by using a multiscale hybrid method, coupling molecular dynamics and hydrodynamic. The temperature of the polymeric liquid rapidly increases due to viscous heating once the drive force exceeds a certain threshold value, and the rheological properties drastically change at around the critical drive force. A remarkable observation is the re-entrant transition in the stress-optical relation at this threshold point.

## [03368] Simulation of multiphase flows based on Lagrangian methods

**Format :** Talk at Waseda University

**Author(s) :** Xin Bian (Zhejiang University)

**Abstract :** We study dynamics of a solid particle, a droplet, a vesicle, and a red blood cell (RBC) suspended in a Newtonian fluid, respectively. These four systems share common features, while distinct behaviors are also very

apparent. We employ the smoothed particle hydrodynamics (SPH) method to solve the matrix fluid universally, but deal with the suspended object differently. We investigate their rich behaviors in Couette/Poiseuille flows.

## [03717] Lagrangian Heterogeneous Multiscale Methods: A generalized multiphysics model for complex fluids with memory

**Format :** Talk at Waseda University

**Author(s) :** Nicolas Moreno (Basque Center for Applied Mathematics)Marco Ellero (Basque Center for Applied Mathematics)

**Abstract :** We present a Lagrangian multiscale/multiphysics framework for modeling complex fluids in various flow configurations. Our method employs Smoothed Dissipative Particle Dynamics (SDPD) to model fluids at both micro and macro scales, allowing us to incorporate complex physical models such as polymer solutions and multiphase flows. The method accurately captures stresses and enables the simulation of mixed flows. We validate the framework with benchmark configurations for Newtonian and non-Newtonian fluids, demonstrating its effectiveness in modeling complex fluids at both scales. Our methodology provides a natural link between macro and microscales and accounts for memory effects, resulting in a richer fluid response at the continuum.

00435 (3/3) : 4E @D101 [Chair: Momoji Kubo]

## [05555] Moisture-induced weakening of adhesion between polymers and metals

**Format :** Talk at Waseda University

**Author(s) :** Shuji Ogata (Nagoya Institute of Technology)

**Abstract :** Adhesive bonding has attracted renewed interest from the manufacturing industry due to its role in creating composite materials and multimaterial designs with the desired arrangements of polymers and metals. In the present work, we theoretically addressed a fundamental problem of the moisture-induced adhesion weakening between polymers (or resin) and metal from a novel viewpoint of (de)protonation of them in water.

## [03509] Modelling and Simulation of Capillary Origami in Three Dimensions

**Format :** Talk at Waseda University

**Author(s) :** Zhixuan Li (National University of Singapore)Weiqing Ren (National University of Singapore)

**Abstract :** Capillary origami involves folding a planar object into a 3D structure using capillary force, and has many important applications such as the fabrication of microelectromechanical systems. In this work, we propose a three-dimensional model of the droplet-on-sheet system with a pinned contact line. The system energy consists of interfacial energies caused by surface tensions and the elastic energy of the thin sheet given by nonlinear Koiter's model. We derive the governing equations of the static equilibrium using a variational approach. We then propose a numerical algorithm to find the equilibrium via a relaxation dynamics. We use the subdivision element method for discretization of the sheet, which provides  $C^1 \cap H^2$  basis functions, and a modified area-minimizing functional for maintaining the mesh quality of the discrete droplet surface. Our numerical simulations demonstrate first-order and second-order convergence in time and space, respectively, and are in good agreement with physical experiments. Specifically, for a triangular sheet, we present phase diagrams of folding, which exhibit rich and fully three-dimensional behaviors not captured by previous two-dimensional models. Our results provide new insights into the mechanics of capillary folding and can inform the design of microfabrication techniques.

## [04590] Multiscale simulation of a polymer melt flow between two coaxial cylinders under nonisothermal conditions

**Format :** Talk at Waseda University

**Author(s) :** Takashi Taniguchi (Kyoto University)Takeshi Sato (Kyoto University)Yuji Hamada (Kyoto University)

**Abstract :** We successfully extend a multiscale simulation (MSS) method to nonisothermal wellentangled polymer melt flows between two coaxial cylinders. In the multiscale simulation, the macroscopic flow system is connected to a number of microscopic systems through the velocity gradient tensor, stress tensor and temperature. At the macroscopic level, in addition to the momentum balance equation, we consider the energy balance equation, where heat generation plays an important role not only in the temperature distribution but also in the flow profile.

## [05592] Flow-type dependent rheologies and multiscale simulations

**Format :** Talk at Waseda University

**Author(s) :** Giulio Giuseppe Giusteri (University of Padua)Francesca Tedeschi (University of Padua)Maria Lukáčová-Medvid'ová (Johannes Gutenberg University of Mainz)Leonid Yelash (Johannes Gutenberg University of Mainz)

**Abstract :** The importance of taking into consideration the dependence on the local flow type of the response of non-Newtonian fluids in multiscale data-driven simulations will be highlighted. A framework to organize data in mixed flows and reconstruct the stress tensor will be reviewed. Then, an algorithm to take into account the flow-type dependence in a consistent way will be presented by discussing paradigmatic planar flows implied by data obtained with a FENE-type model for polymer chains.

## [00436] Coupled dynamical systems: from data analysis to biomathematics

**Session Time & Room :** 2C (Aug.22, 13:20-15:00) @F308

**Type :** Proposal of Minisymposium

**Abstract :** This minisymposium presents recent results in the study of coupled systems, from small groups of elements (neurons, cardiomyocytes, chemical reactions, and so on) to large ones. We propose different lines of study from data analysis techniques to dynamical systems theory approaches to deal with these problems from isolated systems to coupled systems .

**Organizer(s) :** Roberto Barrio, Hiroyuki Kitajima, Valeriy Makarov, Ivan Tyukin

**Classification :** 37Cxx, 34Cxx, 92B05, Dynamical systems; Biomathematics

**Minisymposium Program :**

00436 (1/1) : 2C @F308 [Chair: Roberto Barrio]

## [03097] Fractal dimension of multidimensional biological recordings

**Format :** Talk at Waseda University

**Author(s) :** Valeri A. Makarov (Universidad Complutense de Madrid)

**Abstract :** A linear mixture model can describe multisite LFPs, EEG, and MEG recordings. The fractal dimension (FD) of such multidimensional data can measure the complexity of different brain states. However, the local stationarity, the data's high dimension, and noise limit the assessment of FD from raw data. We discuss theoretical principles and methods derived from the model enabling accurate estimation of the FD, and illustrate them on synthetic and biological data.

## [03895] Lyapunov-like characterization of ghost and weak attractors in complex dynamical systems

**Format :** Talk at Waseda University

**Author(s) :** Ivan Y Tyukin (King's College London)Alexander N Gorban (University of Leicester)Roqaiyah Alsolami (University of Leicester)Tatiana Tyukina (University of Leicester)

**Abstract :** In this talk we discuss the problem of identifying and formally characterizing ghost and weak attractors in complex dynamical systems governed by systems of coupled nonlinear ordinary differential equations. We present a set of conditions enabling to determine if an equilibrium is a weak attractor in terms of the corresponding Jacobian and Hessian matrices. We show how these results can be used to constructively define and determine the existence of ghost attractors in such systems.

## [03442] Flip-flip bifurcations in mathematical cardiac systems with and without symmetry

**Format :** Talk at Waseda University

**Author(s) :** Hiroyuki Kitajima (Kagawa University)

**Abstract :** We study the intersection of double-flip (period-doubling) bifurcations in a parameter plane. We derive normal forms for discrete-time and continuous-time systems. Using these normal forms, we clarify the bifurcation structure around the flip-flip bifurcation point. We apply these analytical results to a system of coupled ventricular cell models. We make the simplest model for generating discordant alternans and clarify that two parameters play key roles in generating discordant alternans.

## [03235] Generation of early afterdepolarizations in cardiomyocytes: Fast-slow and bifurcation analysis

**Format :** Talk at Waseda University

**Author(s) :** Roberto Barrio (University of Zaragoza, Spain)Jorge Jover-Galtier (University of Zaragoza)M. Angeles Martinez (University of Zaragoza)Lucia Perez (University of Oviedo)Sergio Serrano (University of Zaragoza)Esther Pueyo (University of Zaragoza)

**Abstract :** We analyze the dynamical mechanisms underlying the formation of arrhythmogenic early afterdepolarizations (EADs) in the cardiomyocyte models of Sato et al. (a biophysically detailed model of dimension 27) and Luo-Rudy (dimension 3). Based on a comparison of the two models, with detailed bifurcation analysis using continuation techniques and using a fast-slow decomposition in the simple model and numerical explorations in the complex model, we propose a conjectured scheme of the formation of EADs that fits well with electrophysiological experimental data on EAD generation.

## [00437] Climate Risks: From Modelling to Applications

**Session Time & Room :**

00437 (1/2) : 3D (Aug.23, 15:30-17:10) @A510

00437 (2/2) : 3E (Aug.23, 17:40-19:20) @A510

**Type :** Proposal of Minisymposium

**Abstract :** There is an increasing awareness of the urgency required to combat climate change and environmental pollution from central governments, researchers, and the industry around the world. Over 130 countries have committed to carbon neutrality targets in various forms, representing approximately 80% of the world population and 90% of the world's GDP. This shift in public attention is particularly relevant to our economic and financial systems in several aspects. This minisymposium discusses how to model and measure climate risks, their implications for corporate decisions, credit risks, and supply chain risks, how to green investing, and how to regulate the climate emissions market. Overall, these progresses allow researchers, regulators, and other stakeholders to improve their insights into the climate transitional risk to the economy, which will enable society to design policies and strategies to help allocate resources for carbon-neutral goals.

**Organizer(s) :** Emmanuel Gobet, Ruixun Zhang, Florian Bourgey

**Classification :** 91B05, 91B70, 91B74, 86A08, 93E03, Climate Risks; Economic and Financial Systems

**Minisymposium Program :**

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00437 (1/2) : 3D @A510 [Chair: Emmanuel Gobet, Ruixun Zhang, Florian Bourgey]

## [01677] Optimal ecological transition path of a credit portfolio distribution, based on Multidate Monge-Kantorovich formulation

**Format :** Talk at Waseda University

**Author(s) :** Emmanuel Gobet (Ecole Polytechnique)Clara Lage (Ecole polytechnique and Univ. Lyon1)

**Abstract :** Accounting for climate transition risks is one of the most important challenges in the transition to a low-carbon economy. Banks are encouraged to align their investment portfolios to CO<sub>2</sub> trajectories fixed by international agreements, showing the necessity of a quantitative methodology to implement it. We propose a mathematical formulation for this problem and a multistage optimization criterion for a transition between the current bank portfolio and a target one. The optimization problem combines the Monge-Kantorovich formulation of optimal transport, for which the cost is defined according to the financial context, and a credit risk measure. We show that the problem is well-posed, and can be embedded into a saddle-point problem for which Primal-Dual algorithms can be used. We design a numerical scheme that is able to solve the problem in available time, with nice scalability properties according to the number of decision times; its numerical convergence is analysed. Last we test the model using real financial data, illustrating that the optimal portfolio alignment may differ from the naive interpolation between the initial portfolio and the target.

## [01674] Optimal Dynamic Contracts and Environmental Pollution

**Format :** Talk at Waseda University

**Author(s) :** Jerome Detemple (Boston University)Hao Xing (Boston University)

**Abstract :** We examine optimal dynamic contracts when production generates harmful pollution. We derive optimal consumption, effort and environmental investment of the agent and solve for the optimal contract offered by the principal. We then solve for a stationary pollution equilibrium in an economy with a continuum of polluting firms. The optimal contract rewards for financial performance and self-pollution mitigation. We study the impact of model parameters on contractual structure, managerial decisions, and the stationary pollution distribution.

## [05305] Optimal Impact Portfolios with General Dependence and Marginals

**Format :** Talk at Waseda University

**Author(s) :** Andrew Lo (MIT)Lan Wu (Peking University)Ruixun Zhang (Peking University)Chaoyi Zhao (Peking University)

**Abstract :** Impact investing typically involves ranking and selecting assets based on a non-financial impact factor, such as the environmental, social, and governance (ESG) score and the prospect of developing a disease-curing drug. We develop a framework for constructing optimal impact portfolios and quantifying their financial performances. Under general bivariate distributions of the impact factor and residual returns from a multi-factor asset-pricing model, the construction and performance of optimal impact portfolios depend critically on the dependence structure (copula) between the two. We derive a general representation theorem to characterize the distribution of induced order statistics (returns of impact-ranked assets), which allows us to explicitly and efficiently compute the optimal portfolio weights under any copula. The optimal weights depend on the tail characteristics of the copula, as well as whether the marginal distribution of residual returns is skewed or heavy-tailed. Our framework requires the estimation of only a constant number of parameters as the number of assets grows, providing a more regularized and robust approach compared to traditional Markowitz portfolios.

## [01585] Using NLP to Analyze Corporate Communication

**Format :** Online Talk on Zoom

**Author(s) :** Markus Leippold (University of Zurich)

**Abstract :** Corporate climate disclosures are considered an essential prerequisite to managing climate-related financial risks. At the same time, current disclosures are imprecise, inaccurate, and greenwashing-prone. We introduce a deep learning approach to enable comprehensive climate disclosure analyses by fine-tuning the climateBert model. From 14,584 annual reports of the MSCI World index firms from 2010 to 2020, we extract the amount of cheap talk, defined as the share of precise versus imprecise climate commitments. We then test various hypotheses by linking three different climate initiatives, namely the Task Force on Climate-Related Financial Disclosure, the Science-Based Targets Initiative, and the Climate Action 100+, to the economic channels of signaling, credibility, and active engagement. In particular, we ask whether these initiatives decrease cheap talk by disciplining companies in how they define and disclose actionable climate commitments in their annual reports.

00437 (2/2) : 3E @A510 [Chair: Emmanuel Gobet, Ruixun Zhang, Florian Bourgey]

## [01328] When Green Investors Are Green Consumers

**Format :** Talk at Waseda University

**Author(s) :** Olivier David Zerbib (EDHEC)Maxime Sauzet (Boston University)

**Abstract :** We introduce investors with preferences for green assets to a general equilibrium setting in which they also prefer consuming green goods. Their preference for green goods induces consumption premia on expected returns, which counterbalance the green premium stemming from their preferences for green assets. Because they provide a hedge when green goods become expensive, brown assets command lower consumption premia, while green investors allocate a larger share of their portfolios towards them. Empirically, the green-minus-brown consumption premia differential reached 30-40 basis points annually, and contributes to explaining the limited impact of green investing on the cost of capital of polluting firms.

## [01612] Bridging Shared Socioeconomic Pathways of GHG Emission and Credit Risk

**Format :** Talk at Waseda University

**Author(s) :** Florian Bourgey (Bloomberg L.P.)

**Abstract :** We investigate the impact of transition risk on a firm's low-carbon production. As the world is facing global climate change, the Intergovernmental Panel on Climate Change has set the idealized carbon-neutral scenario around

2050. In the meantime, many carbon reduction scenarios, known as Shared Socioeconomic Pathways (SSPs) have been proposed in the literature for different production sectors in a more comprehensive socio-economic context. We consider, on the one hand, a firm that aims to optimize its emission level under the double objectives of maximizing its production profit and respecting the emission mitigation scenarios. Solving the penalized optimization problem provides the optimal emission according to a given SSP benchmark. On the other hand, such transitions affect the firm's credit risk. We model the default time by using the structural default approach. We are particularly concerned with how, by following different SSPs scenarios, the adopted strategies may influence the firm's default probability. We then show how to incorporate physical risk and extend the previous framework to a large-sized portfolio.

### **[01683] On some initial climate change impact models in actuarial science**

**Format :** Online Talk on Zoom

**Author(s) :** Stephane Loisel (ISFA, Universite Lyon 1)

**Abstract :** In this talk, we start by presenting the main sources of uncertainty about the impact of climate change in the insurance industry, and the approaches proposed to model them. We then focus on the impact of physical risk on biometric risks for life insurance and on claims frequency risk in non-life insurance and present work in progress on these two topics.

### **[05370] Optimal carbon tax in the Golosov et al. 2014 DGSE central planning model**

**Format :** Online Talk on Zoom

**Author(s) :** Stéphane Crépey (Université Paris Cité / LPSM)Dounia Essakat (Université Paris Cité / LPSM)Florian Bourgey (Bloomberg L.P.)Noufel Frokha (Université Paris 1)Gauthier Vermandel (Ecole Poytechnique)

**Abstract :** We provide a full analytical solution to the Golosov et al. 2014 optimal control formulation of the carbon tax problem in a DGSE central planning setup. Whereas the original paper was only solving the problem in terms of first order necessary conditions, we derive the value function itself. This gives a direct access to the carbon tax as the derivative of the value function with respect to the Lagrangian parameter associated with the labor constraint.

## **[00441] Intersection between financial economics and optimal control**

**Session Time & Room :**

00441 (1/2) : 1E (Aug.21, 17:40-19:20) @D502

00441 (2/2) : 2C (Aug.22, 13:20-15:00) @D502

**Type :** Proposal of Minisymposium

**Abstract :** Optimal control is widely applied to understand strategic behavior of agents in financial economics. For example, an investor or a household makes investment and consumption decisions, a firm decides production, investment, and financing policies. Optimal control helps to understand these problems in a random environment facing constraints, risk, and uncertainties. Meanwhile, financial applications motivate new forms of control problems. This mini-symposium presents the latest developments in the applications of optimal control in financial economics.

**Organizer(s) :** Scott Robertson, Hao Xing  
**Sponsor :** This session is sponsored by the SIAM Activity Group on Financial Mathematics and Engineering.

**Classification :** 91-10, 91G50, 91G10

**Minisymposium Program :**

00441 (1/2) : 1E @D502 [Chair: Hao Xing]

### **[05612] Asset Pricing with Misallocation**

**Format :** Talk at Waseda University

**Author(s) :** Yan Ji (HKUST)

**Abstract :** We develop an endogenous growth model with heterogeneous firms facing financial frictions, in which misallocation emerges explicitly as a crucial state variable. In equilibrium, misallocation endogenously generates long-run uncertainty about economic growth by distorting innovation decisions, leading to significant welfare losses and risk premia in capital markets. Macroeconomic shocks that affect misallocation are likely to have overly persistent effects on aggregate growth. Using an empirical misallocation measure motivated by the model, we find evidence showing that

misallocation captures low-frequency variations in both aggregate growth and stock returns. Empirically, a two-factor model with market and misallocation factors prices size, book-to-market, momentum, and bond portfolios with an  $R^2$  squared and a mean absolute pricing error close to the Fama-French three-factor model.

### **[03797] An optimal consumption and investment problem for general factor models : Epstein-Zin recursive utility case.**

**Format :** Talk at Waseda University

**Author(s) :** Hiroaki Hata (Hitotsubashi University)

**Abstract :** We consider an optimal consumption and investment problem with Epstein-Zin recursive utility on the finite time horizon. The returns and volatilities of the assets depend on nonlinearly on the factor processes modeled as diffusion process. The problem becomes a standard control problem. We derive the Hamilton-Jacobi-Bellman (HJB) equation and study its solutions. Under some conditions we construct a suitable pair of sub- and super-solution. And, we prove the existence and uniqueness of solution for this HJB equation.

Finally, we show the verification theorem.

### **[05413] Patience is a virtue: optimal investment in the presence of limit order book**

**Format :** Talk at Waseda University

**Author(s) :** Nan Chen (The Chinese University of Hong Kong)Qiheng Ding (The Chinese University of Hong Kong)Chen Yang (The Chinese University of Hong Kong)

**Abstract :** We study an optimal investment problem of a CARA investor trading in a market operated with a limit order book (LOB). The model synergizes three key features of market microstructure: the bid-ask spread, the market depth, and a finite market resilience. Under a Bachelier process for the dynamic of the fundamental value of the asset, we manage to develop explicit characterization through a system of variational inequalities on the investor's optimal trading strategy. A patience index is derived to highlight the importance of trading timing in reconciling several competing goals such as achieving the current optimal risk exposure, incorporating the trading signals about the future, and minimizing trading impact costs.

### **[05411] Why is Cash U-Shape in Firm Size?**

**Format :** Talk at Waseda University

**Author(s) :** Hao Xing (Boston University)Ali Kakhdod (UC Berkeley)Anders Max Reppen (Boston University Questrom School of Business)Tarik Umar (Rice University)

**Abstract :** Cash holdings are U-shaped in firm size. To rationalize this finding, we develop a model of firm dynamics with costly financing allowing for heterogeneous size. Cash is U-shaped in firm size because of decreasing returns to scale and hedging incentives. When a firm is small, cash decreases with size because investment opportunities are better resulting in more aggressive investing. Investing slows as the firm grows, and eventually, cash increases with firm size to hedge larger-scale cash flow shocks. Our model likewise explains why in the data issuance amounts (payout rates) are U-shaped (hump-shaped) in firm size.

00441 (2/2) : 2C @D502 [Chair: Hao Xing]

### **[02868] Debt Maturity Management**

**Format :** Talk at Waseda University

**Author(s) :** Chao Ying (Chinese University of Hong Kong)Yunzhi Hu (UNC)Felipe Varas (Duke)

**Abstract :** This paper studies how a borrower issues long- and short-term debt in response to shocks to the enterprise value. Our theory highlights the tradeoff between commitment and hedging. Short-term debt protects creditors from future dilution and forces the borrower to reduce leverage after negative shocks. Long-term debt postpones default and allows the borrower time to recover after a downturn, thereby providing hedging in the upturn.

### **[05611] Nonlinear Dependence and Households' Portfolio Decisions over the Life Cycle**

**Format :** Online Talk on Zoom

**Author(s) :** Wei Jiang (HKUST)Shize Li (HKUST)Jialu Shen (University of Missouri)

**Abstract :** This paper uncovers the nonlinear relationship between earning risk and stock returns, as measured by the between-squares correlation. By incorporating this between-squares correlation into a life-cycle model, we demonstrate that it lowers households' participation rate and generates moderate risky asset holdings. We identify two pathways through which the between-squares correlation affects portfolio choices: the skewness and kurtosis channels. The extent to which these channels dominate each other depends on the level of between-squares correlation, leading to a nonlinear

relationship between this variable and household decisions. Our empirical studies support the model's predictions. Moreover, we find that ignoring between-squares correlations leads to substantial welfare loss and contributes to increasing wealth inequality.

## [04014] Dynamic Equilibrium with Insider Information and General Uninformed Agent Utility

**Format :** Online Talk on Zoom

**Author(s) :** Scott Robertson (Boston University) Jerome Detemple (Boston University)

**Abstract :** In this talk, we establish the existence of equilibrium in the presence of both asymmetric information and general preferences for the uninformed agent. Specifically, there is an insider who possesses a private signal about the terminal value of the traded asset, and an uninformed agent who possesses no private signal. While the insider has CARA (exponential) preferences, the uninformed agent's preferences are described by a general utility function defined for positive wealth. The terminal value of the traded asset is a function of a time homogeneous diffusion. In this setting, and under mild conditions on the diffusion, terminal payoff function, and uninformed preferences, we establish existence of a partially revealing equilibrium, where a market signal is communicated to all agents at time zero. Additionally, the equilibrium is a rational expectations equilibrium in the univariate case. As the uninformed agent preferences are general, we are able to obtain sensitivity of the asset price, volatility, and market price of risk, to the uninformed agent's initial endowment, as we will show through examples. This is joint work with Jerome Detemple of Boston University.

## [00444] Complex Systems: Advances in Theory and Applications

**Session Time & Room :**

00444 (1/2) : 1C (Aug.21, 13:20-15:00) @G304

00444 (2/2) : 1D (Aug.21, 15:30-17:10) @G304

**Type :** Proposal of Minisymposium

**Abstract :** Many social, biological, and technological networks display non-trivial features, with complicated structures patterns of connection. Well-known classes of complex networks are scale-free and small-world networks. The study of complex networks is growing and many new aspects of network structures attract attention in mathematics, physics, electric power systems, biology, climate, computer science, sociology, epidemiology, and others. There is also a wide range of practical issues including Coupled networks and cyber-physical networks; Networked control; Multi-agent systems: Synchronization phenomena; Complex engineering design, including communication networks, power grids, electronic circuits, biomedical systems, software systems; Biological systems, neural networks, disease transmission.

**Organizer(s) :** Maciej Ogorzalek

**Classification :** 05C82, 68Q06, 68M10, 91D10

**Minisymposium Program :**

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00444 (1/2) : 1C @G304 [Chair: Guanrong Chen]

## [01282] Time Series Analysis with Machine Learning

**Format :** Talk at Waseda University

**Author(s) :** Michael Small (University of Western Australia) Braden John Thorne (University of Western Australia) Eugene Tan (University of Western Australia) Débora Corrêa (University of Western Australia) Ayham Zaitouny (University of Western Australia) Thomas Stemler (University of Western Australia)

**Abstract :** Machine learning is widely applied to model dynamical systems and make predictions. Instead of doing this, We will introduce the concept of Reservoir Time Series Analysis - using a particular flavour of machine learning (reservoir computing) to represent the state of a dynamical system and characterise the dynamical evolution of that state. How much can we infer about the changing behaviour of a system from the internal representation of these states within a reservoir machine learning model? A second strategy within machine learning for time series analysis is to use the machine learning model as a proxy for the original dynamics - but how well do such models capture chaotic dynamics? I will show via some short examples that persistent homology can be used as an effective tool to quantify that structure. These methods will be illustrated with applications to machine vibration and pump cavitation in industrial processes.

## [01306] On constructing directed networks from multivariate time series

**Format :** Talk at Waseda University

**Author(s) :** Tomomichi Nakamura (University of Hyogo)Toshihiro Tanizawa (Toyota)

**Abstract :** We consider a problem of constructing networks for multivariate time series. To construct networks from multivariate time series, we first need to detect relationships among them. However, it is difficult, because the relationships among multivariate time series are diverse. The time series might contain components that have large differences in the amplitude and the time scales of the fluctuations. We consider this problem using the transfer entropy, one of the common techniques for detecting causal relationships and Reduced Auto-Regressive (RAR) model, an information theoretic reduction of auto-regressive model.

## [05563] Optimal network synchronization and a higher-order topological approach

**Author(s) :** Maciej Ogorzalek (Jagiellonian University)Guanrong (Ron) Chen (City University of Hong Kong )

**Abstract :** In this talk, we will discuss the optimal network synchronization problem. The totally homogenous network approach will be reviewed, and a higher-order topological approach will be introduced, with some preliminary results reported.

## [01273] Evaluating the Network Robustness: A Convolutional Neural Network Approach

**Format :** Online Talk on Zoom

**Author(s) :** Yang Lou (Osaka University)Junli Li (Sichuan Normal University)Guanrong Chen (City University of Hong Kong)

**Abstract :** Evaluating network robustness by attack simulations is computationally time-consuming. In this talk, a convolutional neural network (CNN)-based robustness estimation is presented, which has three schemes, including the straightforward scheme, the learning feature-assisted scheme, and the pyramid pooling-assisted scheme. Experimental studies demonstrate that: 1) the prediction error is low; 2) the runtime is significantly lower than that of attack simulations; and 3) it provides a good indicator for robustness, better than the classical spectral measures.

00444 (2/2) : 1D @G304 [Chair: Maciej Ogorzalek]

## [01264] Adaptive Finite-Time Output Consensus for Fractional-Order Complex Networks With Multiple Output Derivative Couplings

**Format :** Talk at Waseda University

**Author(s) :** Chenguang Liu (Beihang University)Qing Gao (Beihang University)Jinhu Lu (Beihang University)

**Abstract :** This paper delves into the adaptive finite-time output consensus (FTOC) problem for a multiple output derivative coupled fractional-order complex network (MODCFOCN). Based on the properties of the Gamma function and the fractional derivative, a FTOC criterion for the MODCFOCN is derived by designing an appropriate adaptive output-feedback controller. Finally, a numerical example is utilized to substantiate the effectiveness of the acquired FTOC results and the devised adaptive output-feedback controller.

## [01255] Optimizing 3D Complex Networks on chip

**Format :** Talk at Waseda University

**Author(s) :** Maciej Ogorzalek (Jagiellonian University)Katarzyna Grzesiaak-Kopec (Jagiellonian University)

**Abstract :** Current generations of integrated circuits can contain billions of transistors and extremely complicated interconnect network the length of which goes into dozens of kilometers – all these placed in an extremely small physical volume.

For the correct operation of the circuit placement of elements and building blocks and design of interconnect has to be done in optimal or quasi-optimal way satisfying also several types of constraints. Mathematical models of complex networks can play a significant role in the design and AI-based methodologies can be used for finding good/quasi-optimal solution in reasonable time.

## [01268] Machine Learning for Detecting Internet Traffic Anomalies

**Format :** Online Talk on Zoom

**Author(s) :** Ljiljana Trajkovic (Simon Fraser University )Ljiljana Trajkovic (Simon Fraser University)

**Abstract :** Border Gateway Protocol (BGP) enables the Internet data routing. BGP anomalies may affect the Internet connectivity and cause routing disconnections, route flaps, and oscillations. Hence, detection of anomalous BGP routing dynamics is a topic of great interest in cybersecurity. Various anomaly and intrusion detection approaches based on

machine learning have been employed to analyze BGP update messages collected from RIPE and Route Views collection sites. Survey of supervised and semi-supervised machine learning algorithms for detecting BGP anomalies and intrusions is presented. Deep learning, broad learning, and gradient boosting decision tree algorithms are evaluated by creating models using collected datasets that contain Internet worms, power outages, and ransomware events.

## [01280] Model for estimating unconfirmed COVID-19 cases and multiple waves of pandemic progression

**Format :** Talk at Waseda University

**Author(s) :** Choujun Zhan (South China Normal University)Chi K. Tse (City University of Hong Kong)

**Abstract :** The novel coronavirus disease 2019 (COVID-19), caused by severe acute respiratory syndrome coronavirus 2 (SARS-CoV-2), has unique epidemiological characteristics that include presymptomatic and asymptomatic infections, resulting in a large proportion of infected cases being unconfirmed, including patients with clinical symptoms who have not been identified by screening. These unconfirmed infected individuals move and spread the virus freely, presenting difficult challenges to the control of the pandemic. To reveal the actual pandemic situation in a given region, a simple dynamic susceptible-unconfirmed-confirmed-removed (D-SUCR) model is developed taking into account the influence of unconfirmed cases, the testing capacity, the multiple waves of the pandemic, and the use of nonpharmaceutical interventions. Using this model, the total numbers of infected cases in 51 regions of the USA and 116 countries worldwide are estimated, and the results indicate that only about 40% of the true number of infections have been confirmed. In addition, it is found that if local authorities could enhance their testing capacities and implement a timely strict quarantine strategy after identifying the first infection case, the total number of infected cases could be reduced by more than 90%. Delay in implementing quarantine measures would drastically reduce their effectiveness.

## [00448] Particle based methods

**Session Time & Room :**

00448 (1/2) : 1C (Aug.21, 13:20-15:00) @E818

00448 (2/2) : 1D (Aug.21, 15:30-17:10) @E818

**Type :** Proposal of Minisymposium

**Abstract :** Predictions of the state or parameter of a system of interest that is subject to some type of stochastic noise are typically achieved by estimating the associated density. Yet this approach becomes highly challenging for extended state and parameter spaces and if the unknown density is non-parametric. State of the art methods are designed to use a Monte Carlo type empirical estimation often referred to as an ensemble or particle filter. Here we will explore theoretical and algorithmic advances of these methods in the context of data assimilation and classical inverse problems.

**Organizer(s) :** Matei Hanu, Jana de Wiljes

**Classification :** 68Txx, 60Gxx, 62Fxx, Data assimilation, Inverse Problems, Machine Learning

**Minisymposium Program :**

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00448 (1/2) : 1C @E818 [Chair: Jana de Wiljes]

## [02827] Constrained sampling

**Format :** Talk at Waseda University

**Author(s) :** Xin Tong (National University of Singapore)

**Abstract :** Sampling-based inference and learning techniques, especially Bayesian inference, provide an essential approach to handling uncertainty in machine learning (ML). As these techniques are increasingly used in daily life, it becomes essential to safeguard the ML systems with various trustworthyrelated constraints, such as fairness, safety, interpretability. We propose a family of constrained sampling algorithms which generalize Langevin Dynamics (LD) and Stein Variational Gradient Descent (SVGD) to incorporate a moment constraint or a level set specified by a general nonlinear function. By exploiting the gradient flow structure of LD and SVGD, we derive algorithms for handling constraints, including a primal-dual gradient approach and the constraint controlled gradient descent approach. We investigate the continuous-time mean-field limit of these algorithms and show that they have  $O(1/t)$  convergence under mild conditions.

## [03107] Subsampling in ensemble kalman inversion

**Format :** Talk at Waseda University

**Author(s) :** Matei Hanu (Free University of Berlin)Jonas Latz (Heriot-Watt-University)Claudia Schillings (Free University of Berlin)

**Abstract :** The Ensemble Kalman Inversion (EKI) is an efficient, gradient-free optimisation method to estimate

unknown parameters in an inverse setting. For large data sets, the EKI becomes computationally infeasible as the data misfit needs to be evaluated for each particle in each iteration.

Randomised algorithms can successfully overcome this issue by using only a random subset of the data in each iteration, so-called subsampling techniques.

In this talk we present subsampling-techniques within Ensemble Kalman Inversion.

## [03842] Ensemble Inference Methods for Models with Noisy and Expensive Likelihoods

**Format :** Talk at Waseda University

**Author(s) :** Marie-Therese Wolfram (University of Warwick) Andrew Stuart (California Institute of Technology) Andrew Duncan (Imperial College London) Oliver Dunbar (California Institute of Technology)

**Abstract :** This talk concerns interacting particle systems to solve inverse problems where the forward model evaluations present rapid fluctuations over the smoothly varying quantity of interest. After comparing the performance of ensemble Kalman methods (EKS) and Langevin-based methods (ELS) using formal multiscale analysis, we introduce a new class of algorithms, named ensemble Gaussian process samplers, which combine the main benefits of both approaches while avoiding their flaws.

## [04379] Projected ensemble data assimilation

**Format :** Talk at Waseda University

**Author(s) :** Svetlana Dubinkina (VU Amsterdam) Jana de Wiljes (University of Potsdam)

**Abstract :** Ensemble data assimilation is unable to reduce the error estimate for high-dimensional systems when used with a small ensemble. A typical remedy is dimension reduction by localization. Though localization reduces the error substantially for both linear and nonlinear data-assimilation methods, the former ones considerably outperform the latter ones in quasi-linear regimes. We propose a further dimension reduction based on projection and show numerically considerable error decrease when used with small ensemble.

00448 (2/2) : 1D @E818 [Chair: Matei Hanu]

## [04587] Alternatives to Monte Carlo based sampling and high dimensional integration

**Format :** Talk at Waseda University

**Author(s) :** Sahani Pathiraja (University of New South Wales)

**Abstract :** Monte Carlo is a fundamental component of popular methods for uncertainty quantification and Bayesian inference. However, Monte Carlo based techniques are often inefficient in high dimensions, representing distributional tails and in complex time-dependent systems. This is in part due to the reliance on points (i.e. delta functions) to approximate distributions. We numerically and analytically investigate the performance of various sampling techniques that make use of alternatives to delta functions and compare to standard Monte Carlo.

## [05018] Mixtures of Gaussian Process Experts with SMC<sup>2</sup>

**Format :** Talk at Waseda University

**Author(s) :** Lassi Roininen (LUT University)

**Abstract :** Gaussian processes are a key component of many flexible statistical and machine learning models. However, they exhibit cubic computational complexity and high memory constraints due to the need of inverting and storing a full covariance matrix. To circumvent this, mixtures of Gaussian process experts have been considered where data points are assigned to independent experts, reducing the complexity by allowing inference based on smaller, local covariance matrices. Moreover, mixtures of Gaussian process experts substantially enrich the model's flexibility, allowing for behaviors such as non-stationarity, heteroscedasticity, and discontinuities. In this work, we construct a novel inference approach based on nested sequential Monte Carlo samplers to simultaneously infer both the gating network and Gaussian process expert parameters. This greatly improves inference compared to importance sampling, particularly in settings when a stationary Gaussian process is inappropriate, while still being thoroughly parallelizable.

## [05073] Eulerian calibration for stochastic transport models

**Format :** Talk at Waseda University

**Author(s) :** Oana Andrea Lang (Imperial College London)

**Abstract :** In this talk I will talk about a new probabilistic approach for calibrating a general class of stochastic nonlinear fluid dynamics models. A key step for ensuring the successful application of the combined stochastic parameterisation and data assimilation procedure is the “correct” calibration of stochastic model parameters. Currently, most methodologies are based on Lagrangian particle trajectories which are simulated starting from each point on both the physical grid and its refined version. Then the differences between the particle positions are used to calibrate the noise.

part\_1

This is computationally expensive and not fully justified from a theoretical perspective. We currently explore an Eulerian approach based on calibrating the amplitude of the individual noises to obtain an approximate representation of uncertainty that uses a finite set of individual noises, and in this talk I will report on the current advances.

This is joint work with Prof Dan Crisan and Dr Alexander Lobbe (Imperial College London).

## [05209] Can possibility theory help with uncertainty quantification for neural networks?

**Format :** Talk at Waseda University

**Author(s) :** Jeremie Houssineau (University of Warwick)

**Abstract :** We consider an alternative to the Gaussian version of the stochastic weight averaging method (SWAG), an approach to uncertainty quantification in neural networks. It is well accepted that the uncertainty in the parameters of the network is epistemic rather than being induced by randomness, which motivates the use of possibility theory. We will see how possibility theory helps to overcome difficulties with standard Bayesian neural networks and how it leads to an alternative to SWAG.

## [00449] Atomistic simulations in the exascale era

**Session Time & Room :**

00449 (1/3) : 4C (Aug.24, 13:20-15:00) @D407

00449 (2/3) : 4D (Aug.24, 15:30-17:10) @D407

00449 (3/3) : 4E (Aug.24, 17:40-19:20) @D407

**Type :** Proposal of Minisymposium

**Abstract :** The world's very first exascale computer has finally arrived. The first generation of exascale machines will predominantly rely on hybrid architectures where massive numbers of CPUs, GPUs, and specialized hardware accelerators, coexist. Realizing the full potential of such architectures is a formidable task that requires an in-depth rethinking of current approaches. In this mini-symposium, we address the challenges faced by computational materials and chemical science communities. We specifically explore novel techniques, algorithms, and methodologies that can extend the time and length scales of atomistic simulations using exascale hardware.

**Organizer(s) :** Joshua Finkelstein, Danny Perez, Emanuel Rubensson, Tony Lelièvre

**Classification :** 82M37, 81-10, 68W10, 65C05, 65Y20

**Minisymposium Program :**

00449 (1/3) : 4C @D407 [Chair: Joshua Finkelstein]

## [01608] Quantum Materials Simulations at the Nexus of Exascale Computing, Artificial Intelligence, and Quantum Computing

**Format :** Talk at Waseda University

**Author(s) :** Aiichiro Nakano (University of Southern California)

**Abstract :** Computing landscape is evolving rapidly. Exascale computers have arrived, and quantum supremacy has been demonstrated for several problems, while artificial intelligence (AI) is transforming every aspect of science and engineering. Atomistic simulations at the exa-quantum-AI nexus are revolutionizing quantum materials research. I will describe research and education on atomically thin two-dimensional and other quantum materials using our AI and quantum-computing enabled exascale materials simulator (AIQ-XMaS). Specifically, I will describe (1) self-assembly of layered material metastructures for scalable and robust manufacturing of quantum emitters for future quantum information science and technology; and (2) excited-state neural-network quantum molecular dynamics (NNQMD) trained by first-principles nonadiabatic quantum molecular dynamics (NAQMD) to prove the exciting concept of picosecond optical, electrical and mechanical control of symmetric breaking in topological ferroelectric skyrmion and skyrmionium for emerging ultralow-power polar topotronics. This research was supported by NSF Future Manufacturing Program, Award 2036359, NSF Cybertraining Program, Award 2118061, and Sony Research Award. Simulations were performed at Argonne Leadership Computing Facility under DOE INCITE and Aurora Early Science programs and at Center for Advanced Research Computing of the University of Southern California.

## [01950] Large scale quantum chemistry with Tensor Processing Units

**Format :** Online Talk on Zoom

**Author(s) :** Ryan Pederson (University of California, Irvine) John Kozlowski (University of California, Irvine) Ruyi Song (Duke University) Jackson Beall (SandboxAQ) Martin Ganahl (SandboxAQ) Markus Hauru (Alan Turing Institute) Adam Lewis (SandboxAQ) Shrestha Basu Mallick (Google LLC) Volker Blum (Duke University) Guifre Vidal (Google LLC)

**Abstract :** We demonstrate the use of Googles cloud-based Tensor Processing Units (TPUs) to accelerate and scale up conventional (cubic-scaling) density functional theory (DFT) calculations. Utilizing 512 TPU cores, we accomplish the largest such DFT computation to date, with 247,848 orbitals, corresponding to a cluster of 10,327 water molecules with 103,270 electrons, all treated explicitly. Our work thus paves the way toward accessible and systematic use of conventional DFT, free of any system-specific constraints, at unprecedented scales.

## [02042] Quantum molecular dynamics using Tensor cores

**Format :** Talk at Waseda University

**Author(s) :** Joshua Finkelstein (Los Alamos National Laboratory) Emanuel H Rubensson (Uppsala) Susan M Mniszewski (Los Alamos National Laboratory) Christian F. A. Negre (Los Alamos National Laboratory) Anders M Niklasson (Los Alamos National Laboratory)

**Abstract :** Tensor cores represent a new form of hardware acceleration specifically designed for deep neural network calculations. They provide extraordinary speed and efficiency but were designed for low-precision tensor contractions. Despite this, we demonstrate how Tensor cores can be applied with high efficiency to the challenging and numerically sensitive problem of quantum-based Born–Oppenheimer molecular dynamics, which requires highly accurate electronic structure optimizations and conservative force evaluations.

## [02949] Recent algorithmic improvements in parallel long-time molecular dynamics

**Format :** Talk at Waseda University

**Author(s) :** Danny Perez (Los Alamos National Laboratory)

**Abstract :** The temporal reach of molecular dynamics is limited by poor parallel strong-scaling: even on exascale computers, direct simulation is expected to remain limited to microseconds. We explore alternative time-wise parallelization schemes that target long-time simulations where multiple trajectory segments are evolved simultaneously and assembled into a unique dynamically correct trajectory. We discuss recent speculative execution and resource-allocation schemes that suggest significant potential scalability enhancements, leading to increased simulation timescales when deployed on massively-parallel computers.

00449 (2/3) : 4D @D407 [Chair: Danny Perez]

## [03771] Adaptive parareal method for the simulation of atomistic defects

**Format :** Online Talk on Zoom

**Author(s) :** Olga Gorynina Tony Lelievre (Ecole des Ponts) Frederic Legoll (Ecole des Ponts) Danny Perez (Los Alamos National Laboratory)

**Abstract :** Molecular dynamics simulations demand extensive computational resources to accurately calculate ensemble averages and dynamical quantities over long trajectories. In this study, we employ an adaptive parareal algorithm to enhance the speed of MD simulations by breaking down time calculations into smaller segments. We focus on the diffusion of a self-interstitial atom in a body-centered cubic tungsten lattice, utilizing LAMMPS molecular dynamics software and employing machine-learned spectral neighbor analysis potentials (SNAP) and embedded-atom method potentials (EAM). The adaptive parareal algorithm, which iteratively refines approximate solutions using parallel fine solvers, demonstrates significant computational gains. The goal of the talk is to highlight the potential of the adaptive parareal algorithm for accelerating MD simulations.

## [04027] Fast, Accurate and Large-scale Ab-initio Calculations for Materials Modeling

**Format :** Talk at Waseda University

**Author(s) :** Vikram Gavini (University of Michigan) Sambit Das (University of Michigan) Phani Motamarri (Indian Institute of Science)

**Abstract :** This talk will present our recent advances towards the development of computational methods and numerical algorithms for conducting fast and accurate large-scale DFT calculations using adaptive finite-element discretization, which form the basis for the recently released DFT-FE open-source code (<https://github.com/dftfedevelopers/dftfe>). The

computational efficiency, scalability and performance of DFT-FE will be presented. Some application problems that highlight the utility of DFT-FE in tackling complex aperiodic systems will be demonstrated.

## [04848] The Chunks and Tasks Matrix Library

**Format :** Talk at Waseda University

**Author(s) :** Emanuel Rubensson (Uppsala University)

**Abstract :** We present the Chunks and Tasks Matrix Library, which is a parallel sparse matrix library able to dynamically take advantage of data locality in matrices to avoid movement of data. The library uses a sparse quadtree representation of sparse matrices and is implemented using the Chunks and Tasks programming model. We demonstrate the scaling capabilities for operations used in large-scale electronic structure calculations, including sparse matrix-matrix multiplication and algorithms for inverse factorization.

## [05282] From Langevin dynamics to kinetic Monte Carlo: mathematical foundations of accelerated dynamics algorithms

**Format :** Online Talk on Zoom

**Author(s) :** Tony LELIEVRE (Ecole des Ponts ParisTech)

**Abstract :** We will discuss models used in classical molecular dynamics, and some mathematical questions raised by their simulations. In particular, we will present recent results on the connection between a metastable Markov process with values in a continuous state space (satisfying e.g. the Langevin or overdamped Langevin equation) and a jump Markov process with values in a discrete state space. This is useful to analyze and justify numerical methods which use the jump Markov process underlying a metastable dynamics as a support to efficiently sample the state-to-state dynamics (accelerated dynamics techniques à la A.F. Voter). It also provides a mathematical framework to justify the use of transition state theory and the Eyring-Kramers formula to build kinetic Monte Carlo or Markov state models.

References:

- G. Di Gesù, T. Lelièvre, D. Le Peutrec and B. Nectoux, Jump Markov models and transition state theory: the Quasi-Stationary Distribution approach, Faraday Discussion, 195, 2016.
- G. Di Gesù, T. Lelièvre, D. Le Peutrec et B. Nectoux, Sharp asymptotics of the first exit point density, Annals of PDE, 5(1), 2019.
- T. Lelièvre, Mathematical foundations of Accelerated Molecular Dynamics methods, In: W. Andreoni and S. Yip (Eds), Handbook of Materials Modeling, Springer, 2018.
- T. Lelièvre, D. Le Peutrec and B. Nectoux, Eyring-Kramers exit rates for the overdamped Langevin dynamics: the case with saddle points on the boundary, <https://arxiv.org/abs/2207.09284>.

00449 (3/3) : 4E @D407 [Chair: Anders Niklasson]

## [05409] Quantum-Mechanical Shadow Born-Oppenheimer Molecular Dynamics for Distributed Computing

**Format :** Talk at Waseda University

**Author(s) :** Anders Niklasson (LANL)

**Abstract :** We present recent developments of quantum-mechanical shadow Born-Oppenheimer molecular dynamics for simulations with tens-of-thousands of atoms using distributed, linear scaling, graph-based electronic structure calculations [Negre, Wall, and Niklasson, J. Chem. Phys. 158, 074108 (2023)].

## [05380] Compressing, resampling and forecasting atomic simulations with descriptor vectors

**Format :** Online Talk on Zoom

**Author(s) :** Thomas D Swinburne (CNRS )

**Abstract :** We show atomic descriptor functions give a metric latent space for atomic simulations, where sparse snapshots can be interpolated and complex transitions (e.g. yielding) can be linearly classified. When descriptors are unimodal, latent trajectories can be resampled and forecasted by a vector autoregressive model, with a Mahalanobis extrapolation grade. The approach is applied to challenging, large-scale simulations of dislocation plasticity. A strategy to optimise resources is proposed, maximising the estimated information yield of additional effort.

## [05479] Structure modeling with large-scale DFT and machine-learning methods

**Format :** Talk at Waseda University

**Author(s) :** Tsuyoshi Miyazaki (National Institute for Materials Science (NIMS))

**Abstract :** To overcome the size limitation of DFT calculations, we have developed a large-scale and linear-scaling DFT code CONQUEST. Using CONQUEST, we can investigate the atomic and electronic structures of large and complex materials containing many thousands of atoms. In this talk, I introduce the recent progress of CONQUEST, together with a newly proposed method to analyze the local atomic structures observed in the DFT-MD simulations of complex systems.

## [00455] Recent Development of Theory and Algorithms of Scientific Machine Learning

**Session Time & Room :**

00455 (1/3) : 1E (Aug.21, 17:40-19:20) @E804

00455 (2/3) : 2C (Aug.22, 13:20-15:00) @E804

00455 (3/3) : 2D (Aug.22, 15:30-17:10) @E804

**Type :** Proposal of Minisymposium

**Abstract :** The “unreasonable effectiveness” of deep learning for massive datasets posed numerous mathematical and algorithmic challenges along the path towards gaining deeper understandings of new phenomena in machine learning. This minisymposium aims at bringing together applied mathematicians interested in the mathematical aspects of deep learning, with diverse background and expertise to modeling high-dimensional scientific computing problems and nonlinear physical systems; the talks reflect the collaborative, multifaceted nature of the mathematical theory and applications of deep neural networks.

**Organizer(s) :** Chunmei Wang, Haizhao Yang

**Classification :** 68Q32, 68T20, 65N21, Machine Learning, Scientific Computing

**Minisymposium Program :**

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00455 (1/3) : 1E @E804 [Chair: Haizhao Yang]

## [05474] Monte Carlo neural networks: Stochastic gradient descent learns random variables

**Format :** Online Talk on Zoom

**Author(s) :** Sebastian Becker (ETH Zurich)Arnulf Jentzen (The Chinese University of Hong Kong, Shenzhen & University of Münster)Marvin Müller (2Xideas Switzerland AG)Philippe von Wurstemberger (ETH Zurich & The Chinese University of Hong Kong, Shenzhen)

**Abstract :** In financial engineering, prices of financial products are computed approximately many times each trading day with (slightly) different parameters in each calculation. Here we introduce a new approximation strategy for such parametric approximation problems where we employ stochastic gradient descent not to train parameters of standard neural networks (NNs) but instead to learn random variables appearing in Monte Carlo approximations. The proposed approach achieves in the tested examples much high approximation precisions than standard NNs.

## [01329] Deep adaptive basis Galerkin method for evolution equations

**Format :** Online Talk on Zoom

**Author(s) :** Yiqi Gu (University of Electronic Science and Technology of China)Michael K. NG (The University of Hong Kong)

**Abstract :** We study deep neural networks (DNNs) for solving high-dimensional evolution equations. Unlike other existing methods (e.g., the least square method) that simultaneously deal with time and space variables, we propose a deep adaptive basis approximation structure. On the one hand, orthogonal polynomials are employed to form the temporal basis to achieve high accuracy in time. On the other hand, DNNs are employed to form the adaptive spatial basis for high dimensions in space.

## [01635] Identifying reaction channels via reinforcement learning

**Format :** Talk at Waseda University

**Author(s) :** Senwei Liang (Lawrence Berkeley Laboratory)

**Abstract :** Reactive trajectories between metastable states are rare yet important in studying reactions. This talk introduces a new method to identify the reaction channels where reactive trajectories occur frequently via reinforcement learning (RL). The action function in RL learns to seek the connective configurations based on reward from simulation. We characterize the reactive channels by data points sampled by shooting from the located connective configurations. These data points bridge stable states and cover most transition regions of interest, enabling us to study reaction mechanism on narrowed regions rather than entire configuration space.

## [03340] Finite Expression Methods for Discovering Pyhsical Laws from Data

**Format :** Online Talk on Zoom

**Author(s) :** chunmei wang (University of Florida)

**Abstract :** The speaker will present the finite expression method (FEX) for discovering the governing equations of data. By design, FEX can provide physically meaningful and interpretable formulas for physical laws compared to black-box deep learning methods. FEX only requires a small number of predefined operators to automatically generate a large class of mathematical formulas. Therefore, compared to existing symbolic approaches, FEX enjoys favorable memory cost and can discover a larger range of governing equations while other methods fail, as shown by extensive numerical tests.

00455 (2/3) : 2C @E804 [Chair: Chunmei Wang]

## [03345] Approximation Theory for Sequence Modelling

**Format :** Talk at Waseda University

**Author(s) :** Qianxiao Li (National University of Singapore)

**Abstract :** In this talk, we present some recent results on the approximation theory of deep learning architectures for sequence modelling. In particular, we formulate a basic mathematical framework, under which different popular architectures such as recurrent neural networks, dilated convolutional networks (e.g. WaveNet), encoder-decoder structures, and transformers can be rigorously compared. These analyses reveal some interesting connections between approximation, memory, sparsity and low rank phenomena that may guide the practical selection and design of these network architectures.

## [03154] Finite Expression Method: A Symbolic Approach for Scientific Machine Learning

**Format :** Talk at Waseda University

**Author(s) :** Haizhao Yang (University of Maryland College Park)

**Abstract :** Machine learning has revolutionized computational science and engineering with impressive breakthroughs, e.g., making the efficient solution of high-dimensional computational tasks feasible and advancing domain knowledge via scientific data mining. This leads to an emerging field called scientific machine learning. In this talk, we introduce a new method for a symbolic approach to solving scientific machine learning problems. This method seeks interpretable learning outcomes in the space of functions with finitely many analytic expressions and, hence, this methodology is named the finite expression method (FEX). It is proved in approximation theory that FEX can avoid the curse of dimensionality in discovering high-dimensional complex systems. As a proof of concept, a deep reinforcement learning method is proposed to implement FEX for learning the solution of high-dimensional PDEs and learning the governing equations of raw data.

## [01880] Discretization Invariant Operator Learning for Solving Inverse Problems

**Format :** Talk at Waseda University

**Author(s) :** Yong Zheng Ong (National University of Singapore)

**Abstract :** Discretization invariant learning aims at learning in the infinite-dimensional function spaces with the capacity to process heterogeneous discrete representations of functions as inputs and/or outputs of a learning model. This talk presents a novel deep learning framework based on integral autoencoders, IAE-Net, for discretization invariant learning. Using IAE-Net, an adaptive training scheme is proposed with different loss functions to train the model. The proposed model is tested with various applications.

## [03159] Deep Adaptive Basis Galerkin Method for Evolution Equations

**Format :** Talk at Waseda University

**Author(s) :** Yiqi Gu (University of Electronic Science and Technology of China)

**Abstract :** We study deep neural networks (DNNs) for solving high-dimensional evolution equations. Unlike other existing methods (e.g., the least square method) that simultaneously deal with time and space variables, we propose a deep adaptive basis approximation structure. On the one hand, orthogonal polynomials are employed to form the temporal basis to achieve high accuracy in time. On the other hand, DNNs are employed to form the adaptive spatial basis for high dimensions in space.

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00455 (3/3) : 2D @E804 [Chair: Haizhao Yang]

## [03467] Multi-scale Neural Networks for High Frequency Problems in Regressions and PDEs

**Format :** Talk at Waseda University

**Author(s) :** Wei Cai (Southern Methodist University)Lizuo Liu (Southern Methodist University)Bo Wang (LCSM(MOE), School of Mathematics and Statistics, Hunan Normal University, Changsha, Hunan, 410081, P. R. China.)

**Abstract :** In this talk, we will introduce multiscale deep neural networks (MscaleDNNs) in order to overcome the spectral bias of deep neural networks when approximating functions with wide-band frequency information. The MscaleDNN uses a radial scaling in the frequency domain, which converts the problem of learning high frequency contents in regression problems or PDE's solutions to one of learning lower frequency functions. As a result, the MscaleDNN achieves fast uniform convergence over multiple scales as demonstrated in solving regression problems and highly oscillatory Navier-Stokes flows. Moreover, a diffusion equation model in the frequency domain is obtained based on the neural tangent kernel, which clearly shows how the multiple scales in the MscaleDNN improves the convergence of the training of neural networks over wider frequency ranges with more scales, compared with a traditional fully connected neural network.

## [05449] Implicit bias in deep learning based PDE solvers

**Format :** Talk at Waseda University

**Author(s) :** Tao Luo (Shanghai Jiao Tong University)Qixuan Zhou (Shanghai Jiao Tong University)

**Abstract :** We will discuss some recent development on the theory of deep learning based PDE solvers. We would like to mention some new ideas on modeling and analysis of such algorithms, especially some related phenomenon observed during the training process. For the theoretical part, both optimization and approximation will be considered.

# [00462] Mathematical and applicable studies on quantum walks

**Session Time & Room :**

00462 (1/2) : 2C (Aug.22, 13:20-15:00) @D405

00462 (2/2) : 2D (Aug.22, 15:30-17:10) @D405

**Type :** Proposal of Minisymposium

**Abstract :** Eigenvalue problems for matrices and spectral theory for unitary operators and self-adjoint operators are important research area of quantum walks. In fact, spectra of time-evolution operators of quantum walks determine the dynamics of quantum walkers. In this minisymposium, we are going to have eight talks on the scattering and the spectral theory for quantum walks as well as eigenvalue problems on quantum walks on finite graphs and related topics. Some of them are going to introduce studies of quantum walks in view of theoretical physics and laser engineering.

**Organizer(s) :** Hisashi Morioka, Etsuo Segawa

**Classification :** 81Q35, 15A18, 47A75, 81Q10, 05C25

**Minisymposium Program :**

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00462 (1/2) : 2C @D405 [Chair: Akito Suzuki]

**[01759] The Ihara expression of graph zeta functions****Format :** Talk at Waseda University**Author(s) :** Ayaka Ishikawa (Yokohama National University)**Abstract :** Konno and Sato showed that the Grover walk corresponds to the Sato zeta function. They also gave the characteristic polynomial of the transition matrix of the Grover walk, using the Ihara expression of the Sato zeta function.

We define the graph zeta function related to the Szegedy walk on a finite graph and give the Ihara expression. The Ihara expression will extend Konno-Sato's result to the Szegedy walk.

**[02778] Topological stability of quantum walks and related****Format :** Talk at Waseda University**Author(s) :** Chris Bourne (Nagoya University)**Abstract :** Quantum walks with additional symmetries may possess topologically protected bound states, meaning these bound states are robust against small perturbations and changes. I will give a gentle mathematical introduction to this phenomenon, which borrows ideas from so-called topological phases of matter. I will also explain how the existence of topological bound states can be detected using a winding number-like formula.**[03296] Spectral mapping theorem for quantum walks on graphs****Format :** Talk at Waseda University**Author(s) :** Kei Saito (Kanagawa University)**Abstract :** Quantum walks (QWs) are well known as a quantum version of random walks, and their time evolution is described by a unitary operator. Segawa, Suzuki(2019) show that the spectrum of the QW is given by that of a self-adjoint operator on the underlying graph. In this talk we reconsider such a spectral mapping theorem from a different perspective and present a relation between the spectrum of QWs and the weighted line matrix.**[05096] The Segawa-Suzuki spectral mapping theorem, revisited****Format :** Talk at Waseda University**Author(s) :** Yohei Tanaka (Gakushuin University)**Abstract :** The Segawa-Suzuki spectral mapping theorem for chiral unitaries is particularly useful when studying spectral properties of chiral symmetric quantum walks. For example, it states that topologically protected bound states can be characterised by elements of the so-called birth and inherited eigenspaces. The purpose of this talk is to show that this characterisation has a yet another interpretation in terms of the real part of a chiral unitary.

00462 (2/2) : 2D @D405 [Chair: Yohei Tanaka]

**[03456] Resonance expansion for quantum walks****Format :** Talk at Waseda University**Author(s) :** Kenta Higuchi (Ehime University)**Abstract :** We study long time behavior of "open" quantum walks by introducing resonances and the resonance expansion. Eigenvalues on the unit circle characterize the localization of quantum walkers. However, an open quantum walk does not have eigenvalues but may have resonances inside the unit circle. Then the decay rate of the quantum walker in any bounded region is described by the modulus of resonances. The eigenstate expansion is generalized to the resonance expansion.**[04207] Spectral scattering theory for quantum walks****Format :** Talk at Waseda University**Author(s) :** Akito Suzuki (Shinshu university)**Abstract :** Spectral scattering theory works to understand the dynamics of quantum walks and obtain the limit distribution of the asymptotic velocity of the walker, which gives a quantum version of the central limit theorem. In this talk, I would like to talk about the recent development of spectral scattering theory for one-dimensional quantum walks.**[04051] Quantum Walk-Based Maze-Solving with Absorbing Holes****Format :** Talk at Waseda University**Author(s) :** Leo Matsuoka (Hiroshima Institute of Technology)Kenta Yuki (Freelancer)Hynek Lavicka (STTech GmbH)Etsuo Segawa (Yokohama National University)**Abstract :** We propose a strategy for finding the shortest path on a bipartite graph maze using a discrete-time quantum walk with absorbing holes. Our numerical analysis shows that the chain of maximum trapped densities detects the

shortest paths in most cases. Furthermore, we discuss the speed of the algorithm and propose a strategy for accelerating it using numerical analysis. Our results offer a potential model for autonomous maze-solving optimization by harnessing natural phenomena.

## [03689] Distinguishability and Complexity in Non-Unitary Boson Sampling Dynamics

**Format :** Online Talk on Zoom

**Author(s) :** Ken Mochizuki (RIKEN)

**Abstract :** We show that quantum walks of many photons are closely related to the boson sampling problem and computational complexity. In addition, we consider non-unitary quantum walks, which correspond to photonic dynamics in open quantum systems with post selection. We clarify that the distribution of photons can approach that of distinguishable particles in the long time limit, which makes the non-unitary boson sampling problem easy.

Ken Mochizuki and Ryusuke Hamazaki, Physical Review Research 5 013177 (2023).

## [00465] Linear and Non-linear Approximation of Curves and Surfaces

**Session Time & Room :**

00465 (1/3) : 1C (Aug.21, 13:20-15:00) @E507

00465 (2/3) : 1D (Aug.21, 15:30-17:10) @E507

00465 (3/3) : 1E (Aug.21, 17:40-19:20) @E507

**Type :** Proposal of Minisymposium

**Abstract :** Approximation techniques are used in problems in which it's required to find unknown functions from a set of known data. This problem appears in physics (solution of hyperbolic PDEs), medicine (medical imaging treatment) or topography (Digital Elevation Models) etc.

Reconstruction based on linear schemes, like splines, have proved to be useful in different application (DEM). However they become ineffective for approximating piecewise smooth functions (shocks in solution of hyperbolic PDEs) or edge-dominated images. For such families, nonlinear schemes may improve the approximation performance.

This MS brings together researchers from the two different communities, with the aim to generate scientific dialogue.

**Organizer(s) :** Francesc Aràndiga

**Classification :** 65D15, 65D07

**Minisymposium Program :**

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00465 (1/3) : 1C @E507 [Chair: Francesc Aràndiga]

## [01862] Stable nonlinear inversion : a general framework for interface reconstruction from cell-average

**Format :** Talk at Waseda University

**Author(s) :** Albert Cohen (Sorbonne Université)

**Abstract :** In this lecture, we present a general framework for solving inverse problem using nonlinear approximation spaces. The main principles build up on the so called Parametrized Background Data Weak method (PBDW) which can be thought as a linear counterpart. As a main and motivating application we discuss the reconstruction of sharp interfaces from cell average at coarse resolutions for which linear methods are known to be ineffective. We discuss the convergence rates of these reconstructions and their optimality.

## [02134] Adaptive Multi-Quadric Interpolation: Applications in Image Compression.

**Format :** Talk at Waseda University

**Author(s) :** Rosa Donat (Universitat de Valencia)Francesc Aràndiga (Universitat de València)Daniela Schenone (Leonardo Sistemi Integrati S.L.R.)

**Abstract :** Multi-Quadric interpolation techniques depend on a shape parameter that has a direct influence on its

accuracy. The computation of the shape parameter can be performed using 'linear' (e.g. data-independent) estimates or by incorporating adaptive techniques, similar to those used in ENO/WENO schemes to maximize the region of accuracy when using piecewise polynomial interpolatory techniques.

We design 2D Prediction operators within Harten's Multiresolution Framework based on non-separable multi-quadric approximation that incorporates a WENO-type selection of the local shape parameter. We explore the compression properties of the resulting MR transformation, and also the combination of these techniques with the construction of edge maps of the image.

## [01772] Reconstructing a Digital Elevation Model from C2 quasi-interpolation

**Format :** Talk at Waseda University

**Author(s) :** Domingo Barrera (University of Granada) Salah Eddargani (University of Rome Tor Vergata) Juan Francisco Reinoso (University of Granada)

**Abstract :** Quasi-interpolation spline in the Bernstein basis is a low-cost computational method for approximating functions or data in one or several variables. Although linked to the degree, regularity and exactness are parameters available to the user. In this contribution we propose to define a one-dimensional quasi-interpolation operator that achieves the optimal approximation order and provides C2 continuous approximants. It will be used to reconstruct a Digital Elevation Model using a tensor product type scheme.

## [01766] Low-degree quasi-interpolation in the Bernstein basis

**Format :** Talk at Waseda University

**Author(s) :** María José Ibáñez (University of Granada) Salah Eddargani (University of Rome Tor Vergata) Sara Remogna (University of Torino)

**Abstract :** Spline quasi-interpolation is an effective tool for approximating functions or data. Usually, the quasi-interpolant is defined as a linear combination of the B-splines of a basis of the linear space in which the approximant is to be constructed. In this contribution we present a procedure for constructing quasi-interpolants by directly defining the coefficients of the expression in the Bernstein basis of its restriction to each subinterval induced by a uniform partition of the real line.

00465 (2/3) : 1D @E507 [Chair: Rosa Donat]

## [01326] A Nonlinear B-spline quasi-interpolation method,

**Format :** Talk at Waseda University

**Author(s) :** Francesc Aràndiga (Universitat de València)

**Abstract :** Quasi-interpolation based on B-spline approximation methods are used in numerous applications. However, we observe that the Gibbs phenomenon appears when approximating near discontinuities. We present nonlinear modifications, based on weighted essentially non-oscillatory (WENO) techniques, of well-known quasi-interpolant methods to avoid this phenomena near discontinuities and, at the same time, maintain the high-order accuracy in smooth regions.

## [01853] Edge adaptive schemes and machine learning for image super-resolution

**Format :** Talk at Waseda University

**Author(s) :** Agustín Somacal (Sorbonne University)

**Abstract :** In image processing Edge-adapted methods are used to reconstruct high-resolution images from coarser cell averages. When images are piece-wise smooth functions, interfaces can be approximated by a pre-specified functional class through optimization LVIRA or specific preprocessing ENO-EA. We extend the ENO-EA approach to polynomials, show two methods to treat vertices and compare with learning-based methods in which an artificial neural network is used to attain the same goal.

## [01411] Univariate subdivision schemes based on local polynomial regression

**Format :** Talk at Waseda University

**Author(s) :** Dionisio F. Yanez (UV)

**Abstract :** The generation of curves and surfaces from given data is a well-known problem in Computer-Aided Design that can be solved by means of subdivision schemes. They are a powerful tool that allows obtaining new data from the initial one using simple calculations. In some real applications, the initial data are given with noise and interpolatory schemes are not adequate to process them. In this talk, we present some new families of binary univariate linear subdivision schemes using weighted local polynomial regression. We study their properties, such as convergence, monotonicity and polynomial reproduction and show some examples.

## [01410] Linear and nonlinear approximation rules arising from optimal denoising

**Format :** Talk at Waseda University

**Author(s) :** Sergio López-Ureña (Universitat de València)

**Abstract :** We explore the design of new linear filter-like methods based on the minimization of the noise variance. But linear methods, when applied to data with large gradients, may lead to some kind of Gibbs phenomenon. To overcome this problem, we combine some of these linear methods in a WENO style to obtain a nonlinear denoising method which handles properly large gradients in the data. Some examples are performed to validate the theoretical results.

00465 (3/3) : 1E @E507 [Chair: Domingo Barrera]

## [01560] A totally C^2 quartic splines defined on mixed macro-structures

**Format :** Online Talk on Zoom

**Author(s) :** Salah Eddargani (University of Rome "Tor Vergata")Domingo Barrera (University of Granada)María José Ibáñez (University of Granada)

**Abstract :** This work deals with the construction of normalized B-splines of degree four and C^2 smooth everywhere on triangulations endowed with mixed splits. The main splits involved herein are Powell-Sabin (6-), and Modified Morgan-Scott (10-) splits. With the help of Marsden identity, a family of C^2 quartic quasi-interpolation splines of optimal orders has been provided.

## [01502] Construction of quadratic and cubic orthogonal wB-spline wavelets

**Format :** Online Talk on Zoom

**Author(s) :** Mohamed Ajeddar (MISI Laboratory, Faculty of Sciences and Technology, University Hassan First, Settat, Morocco.)

**Abstract :** The definition and basic properties of  $\omega$ B-splines, frequently used as primal scaling functions, are introduced, as well as their refinement equation. Then, a method for constructing orthogonal wavelets using  $C^1$  and  $C^2$   $\omega$ B-splines is presented.

## [01492] Algebraic Hyperbolic spline interpolation by means of integral values.

**Format :** Online Talk on Zoom

**Author(s) :** Mohammed Oraiche (Department of Mathematics, University Hassan First, Settat, Morocco.)

**Abstract :** In this paper, a cubic Hermite spline interpolating scheme reproducing both linear polynomials and hyperbolic functions is considered. The interpolating scheme is mainly defined by means of integral values over the subintervals of a partition of the function to be approximated, rather than the function and its first derivative values. The scheme provided is  $C^2$  everywhere and yields optimal order. We provide some numerical tests to illustrate the good performance of the novel approximation scheme.

## [00467] Volatility modeling in finance

**Session Time & Room :**

00467 (1/3) : 4C (Aug.24, 13:20-15:00) @D502

00467 (2/3) : 4D (Aug.24, 15:30-17:10) @D502

00467 (3/3) : 4E (Aug.24, 17:40-19:20) @D502

**Type :** Proposal of Minisymposium

**Abstract :** Volatility is the single most important factor driving the dynamics of financial assets. Volatility modeling has been a very active field of research in the past years. Recent developments include in particular rough volatility, path-dependent volatility, including signature models, as well as designing models that jointly calibrate to S&P 500 and VIX options. This minisymposium aims to present in one place, compare, and bridge different new approaches on volatility modeling. It is our hope that fruitful ideas and collaborations can emerge from it.

**Organizer(s) :** Julien Guyon  
**Sponsor :** This session is sponsored by the SIAM Activity Group on Financial Mathematics and Engineering.

**Classification :** 91-XX, 60-XX, 62-XX, Quantitative finance

**Minisymposium Program :**

00467 (1/3) : 4C @D502 [Chair: Julien Guyon]

part\_1

## [05137] Volatility is (Mostly) Path-Dependent

**Author(s)** : Julien Guyon (Ecole des Ponts ParisTech)Jordan Lekeufack Sopze (University of California, Berkeley)

**Abstract** : Using data, we show that volatility is mostly path-dependent: 90% of the implied volatility of equity indexes is explained endogenously by past index returns thanks to a simple linear model that combined weighted sums of past daily returns and squared returns with different time-shifted power-law weights. It thus suggests a continuous-time Markovian path-dependent volatility model. This model captures key stylized facts of volatility, and fits SPX and VIX smiles well, solving joint SPX/VIX smile calibration problem.

## [05626] The 4-Factor Path-Dependent Volatility Model

**Author(s)** : Julien Guyon (Ecole des Ponts ParisTech)

**Abstract** : The natural Markovian continuous-time version of the empirical path-dependent volatility (PDV) uncovered in [Guyon and Lekeufack, Volatility Is (Mostly) Path-Dependent, 2022] is the 4-Factor PDV model. Two factors describe the short and long dependence of volatility on recent returns (trend), while the two other factors describe the short and long dependence of volatility on recent returns squared (historical volatility). We show that this model, which is inferred from the empirical joint behavior of returns and volatility, captures all the important stylized facts of volatility: leverage effect, volatility clustering, large volatility spikes followed by a slower decrease, roughness at the daily scale, very realistic SPX and VIX smiles, joint calibration, Zumbach effect and time-reversal asymmetry. Being Markovian in low dimension, the model is very easy and fast to simulate. It can easily be enhanced with stochastic volatility (PDSV) to account for exogenous shocks. This is joint work with Jordan Lekeufack.

## [01960] A theoretical analysis of Guyon's toy volatility model

**Format** : Talk at Waseda University

**Author(s)** : Ofelia Bonesini (Imperial College London)Antoine Jacquier (Imperial College London)Chloé Lacombe (Morgan Stanley)

**Abstract** : We provide a thorough analysis of a path-dependent volatility model introduced by Guyon, proving existence and uniqueness of a strong solution, characterising its behaviour at boundary points, providing asymptotic closed-form option prices as well as deriving small-time behaviour estimates.

## [05614] Prediction through Path Shadowing Monte-Carlo

**Format** : Online Talk on Zoom

**Author(s)** : Julien Guyon (Ecole des Ponts ParisTech)Rudy Morel (Ecole Normale Supérieure)

**Abstract** : We introduce a Path Shadowing Monte-Carlo method, which provides prediction of future paths, given any generative model. At a given date, it averages future quantities over generated price paths whose past history matches, or “shadows”, the actual (observed) history. We test our approach using paths generated from a maximum entropy model of financial prices, based on a recently proposed multi-scale analogue of the standard skewness and kurtosis called “Scattering Spectra”. This model promotes diversity of generated paths while reproducing the main statistical properties of financial prices, including stylized facts on volatility roughness. Our method yields state-of-the-art predictions for future realized volatility. It also allows one to determine conditional option smiles for the S&P500. These smiles depend only on the distribution of the price process, and are shown to outperform both the current version of the Path Dependent Volatility model and the option market itself.

00467 (2/3) : 4D @D502 [Chair: Julien Guyon]

## [04506] Understanding how market impact shapes rough volatility

**Author(s)** : Mathieu Rosenbaum (École Polytechnique )Gregoire Szymanski (Ecole Polytechnique)

**Abstract** : We explain the subtle connection between the shape of market impact curves and the rough behavior of the volatility. We particularly focus on the celebrated square-root law and on the role of the participation rate in the price and volatility formation process.

## [04065] Pricing in affine forward variance models

**Format** : Talk at Waseda University

**Author(s)** : Jim Gatheral ( Baruch College, CUNY)

**Abstract** : In affine forward variance (AFV) models, the moment generating function may be expressed as the convolution of the forward variance curve and the solution of an associated convolution integral equation. In the case of the rough Heston model, this convolution integral equation may be solved numerically using the Adams scheme and approximately using a rational approximation. We show that in the general case, AFV models may be simulated

efficiently using a hybrid version of Andersen's QE scheme. We illustrate convergence of the scheme numerically in the special case of the rough Heston model.

## [02829] The rough Hawkes Heston model

**Format :** Talk at Waseda University

**Author(s) :** Sergio Andres Pulido Nino (ENSIIE-LaMME, Evry)Alessandro Bondi (Scuola Normale Superiore di Pisa)Simone Scotti (Universita di Pisa)

**Abstract :** We introduce an extension of the Heston stochastic volatility model that incorporates rough volatility and jump clustering phenomena. In our model, the spot variance is a rough Hawkes-type process proportional to the intensity process of the jump component appearing in the dynamics of the spot variance itself and the log returns. The model belongs to the class of affine Volterra models. In particular, the Fourier-Laplace transform of the log returns and the square of the volatility index can be computed explicitly in terms of solutions of deterministic Riccati-Volterra equations, which can be efficiently approximated using a multi-factor approximation technique. Prices of options on the underlying and its volatility index can then be obtained using Fourier-inversion techniques. We show that a parsimonious setup, characterized by a power kernel and an exponential law for the jumps, is able to simultaneously capture the behavior of the implied volatility smile for both S&P 500 and VIX options. Our findings demonstrate the relevance, under an affine framework, of rough volatility and self-exciting jumps in order to jointly calibrate S&P 500 and VIX smiles.

## [05086] Recent advances on rough volatility

**Format :** Talk at Waseda University

**Author(s) :** Antoine Jacquier (Imperial College London)

**Abstract :** Empirical evidence has recently highlighted that volatility of financial markets was not Markovian, giving rise to a new paradigm called "rough volatility". In this talk, we consider several recent advances in the topic, from a modelling point of view (suggesting interesting extensions of fractional Brownian motion) and from numerical aspects.

00467 (3/3) : 4E @D502 [Chair: Julien Guyon]

## [04764] Does the Term-Structure of Equity At-the-Money Skew Really Follow a Power Law?

**Format :** Talk at Waseda University

**Author(s) :** Mehdi El Amrani-Zirifi (Bloomberg LP)Julien Guyon (Ecole des Ponts ParisTech)

**Abstract :** Using two years of S&P 500, Eurostoxx 50, and DAX data, we empirically investigate the term-structure of the at-the-money-forward (ATM) skew of equity indexes. While a power law (2 parameters) captures the term-structure well away from short maturities, the power law fit deteriorates considerably when short maturities are included. By contrast, 3-parameter shapes such as time-shifted or capped power laws, are shown to fit well regardless of whether short maturities are included or not.

## [04899] Fast exact joint S&P 500/VIX smile calibration in discrete and continuous time

**Format :** Talk at Waseda University

**Author(s) :** Florian Bourgey (Bloomberg L.P.)Julien Guyon (Ecole des Ponts ParisTech)

**Abstract :** We introduce the Newton--Sinkhorn and implied Newton algorithms which significantly speed up the Sinkhorn algorithm that (Guyon, Risk, April 2020) used to build the first arbitrage-free model exactly consistent with S&P 500 and VIX market data. Using a purely forward Markov functional model, we show how to build a continuous-time extension of the previous discrete-time model. We also compute model-free bounds on S&P 500 options that show the importance of taking VIX smile information into account. Extensive numerical tests are conducted.

## [03758] Joint calibration to SPX and VIX options with signature-based models

**Format :** Talk at Waseda University

**Author(s) :** Christa Cuchiero (University of Vienna)Guido Gazzani (University of Vienna)Janka Möller (University of Vienna)Sara Svaluto-Ferro (University of Verona)

**Abstract :** We consider a stochastic volatility model where the dynamics of the volatility are described by linear functions of the signature of a primary process. Under the assumption that this process is polynomial, we can express the log-price and the VIX squared as linear functions of the signature of an (augmented) primary process. This feature can be efficiently used for calibration purposes since the signature samples can be easily precomputed. We also propose a Fourier approach for VIX and SPX options exploiting that the signature of the augmented primary process is an infinite dimensional affine process.

## [03638] Neural Joint SPX/VIX Smile Calibration

**Format :** Talk at Waseda University

**Author(s) :** Scander Mustapha (Princeton University)Julien Guyon (CERMICS, Ecole des Ponts ParisTech)

**Abstract :** We calibrate neural stochastic differential equations jointly to S&P 500 smiles, VIX futures, and VIX smiles. Drifts and volatilities are modeled as neural networks. Minimizing a suitable loss allows us to fit market data for multiple S&P 500 and VIX maturities. A one-factor Markovian stochastic local volatility model is shown to fit both smiles and VIX futures within bid-ask spreads. The joint calibration actually makes it a pure path-dependent volatility model, confirming the findings in [Guyon, 2022, The VIX Future in Bergomi Models: Fast Approximation Formulas and Joint Calibration with S&P 500 Skew].

## [00468] Stochastic Modelling in Finance



**Session Time & Room :** 4D (Aug.24, 15:30-17:10) @D505

**Type :** Proposal of Minisymposium

**Abstract :** The mini-symposium is devoted to the recent developments in stochastic modelling in finance. It will include stochastic modelling of big data in finance, portfolio optimization problems in incomplete stochastic volatility financial markets, driven by both Brownian motion and a jump processes, as well as a Heston 1/2 component and a 3/2 component the state-of-the-art 4/2 stochastic volatility models, and also new modelling involving Parrondo's paradox and its financial applications.

**Organizer(s) :** Anatoliy Swishchuk

**Classification :** 91G15, 91B24, 60H10, 60K15, 60F05

**Minisymposium Program :**

00468 (1/1) : 4D @D505 [Chair: Anatoliy Swishchuk, University of Calgary, Calgary, AB, Canada]

### [01313] Portfolio optimization in the family of 4/2 stochastic volatility models.

**Format :** Online Talk on Zoom

**Author(s) :** Marcos Escobar-Anel (Western University, Department of Statistical and Actuarial Sciences.)

**Abstract :** The state-of-the-art 4/2 stochastic volatility model was recently proposed by Grasselli in 2017 and has gained great attention ever since. This model is a superposition of a Heston (1/2) component and a 3/2 component, bringing the best of the two nested models. This talk gives an overview of recent progress in the application of the model, as well as a multivariate generalization, to portfolio optimization, in particular within expected utility theory. The work includes the study of CRRA and HARA utilities, the presence of consumption, as well as considerations about complete/incomplete markets and ambiguity-aversion. All is complemented with the analysis of wealth-equivalent losses to gain insight into popular suboptimal strategies.

### [01486] Parrondo's paradox and financial applications

**Format :** Online Talk on Zoom

**Author(s) :** Bruno N Remillard (HEC Montreal)

**Abstract :** In this talk, I will start by giving an introduction to Parrondo's paradox, then I will present recent results on this topic, and finally I will talk about financial applications.

### [01304] Optimal portfolio analysis on finite and small-time horizons

**Format :** Online Talk on Zoom

**Author(s) :** Indranil SenGupta (North Dakota State University)

**Abstract :** In this presentation, we consider the portfolio optimization problem in a financial market under a general utility function. We consider an incomplete stochastic volatility market model that is driven by both Brownian motion and jump process. We obtain a closed-form formula for an approximation to the optimal portfolio in a small-time horizon. This is obtained by finding the associated Hamilton-Jacobi-Bellman integro-differential equation and then approximating the value function by constructing appropriate supersolution and subsolution.

### [01292] Stochastic Modelling of Big Data in Finance

**Format :** Talk at Waseda University

**Author(s) :** Anatoliy Swishchuk (University of Calgary)

**Abstract :**

This talk will review some recent results in stochastic modelling of big data in finance, including semi-Markov

modelling, modelling with Hawkes processes, multivariate modelling, to name a few. Numerical results are used to explain, visualize and justify the proposed models, and are based on real data such as LOBster, CISCO, Xetra and Frankfurt markets stocks and other data.

## [00471] Recent Advancements in Electrical Impedance Tomography

### **Session Time & Room :**

00471 (1/2) : 4C (Aug.24, 13:20-15:00) @D515

00471 (2/2) : 4D (Aug.24, 15:30-17:10) @D515

**Type :** Proposal of Minisymposium

**Abstract :** Electrical impedance tomography is an imaging modality based on solving the inverse conductivity problem, in which known boundary voltages and currents are used to reconstruct information about an object's interior. The inversion process is known to be both highly nonlinear and highly ill-posed, and thus provides researchers with an ongoing wealth of interesting problems. The cutting edge of research in EIT includes both theoretical and computational developments, and is relevant to a wide variety of medical and industrial applications. This minisymposium will gather leading experts in EIT along with young researchers to share their new results and insights.

**Organizer(s) :** Melody Alsaker, Samuli Siltanen

**Classification :** 92C55, 35R30, 78A46

### **Minisymposium Program :**

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00471 (1/2) : 4C @D515 [Chair: Samuli Siltanen]

## [04879] A Multithreaded Implementation of the D-bar Algorithm for 2D Functional EIT Imaging

**Format :** Talk at Waseda University

**Author(s) :** Melody Alsaker (Gonzaga University)

**Abstract :** D-bar algorithms for Electrical Impedance Tomography have high computational complexity. Previous attempts at fast D-bar implementations had some limitations: these methods used a parallelization strategy which caused a time delay between data acquisition and reconstruction, and they used coarse spatial meshes with large numbers of CPU cores. Furthermore, data acquisition speed of modern EIT systems has increased, making previously published runtimes out-of-date. In this talk, we present a new multithreaded solution which addresses these problems.

## [02729] New insight into EIT reconstruction using virtual X-rays

**Format :** Talk at Waseda University

**Author(s) :** Siiri Rautio (University of Helsinki)

**Abstract :** We introduce a new reconstruction algorithm for EIT, which provides a connection between EIT and X-ray tomography. We divide the ill-posed and nonlinear inverse problem of EIT into separate steps. We start by calculating “virtual” X-ray projection data from the DN map. Then, we perform algebraic operations and integration, ending up with a blurry Radon sinogram. We use neural networks to deconvolve the sinogram and finally, we compute a reconstruction using the inverse Radon transform.

## [04009] Combining electrical impedance tomography and machine learning for stroke classification

**Format :** Talk at Waseda University

**Author(s) :** Juan Pablo Agnelli (National University of Córdoba)

**Abstract :** There are two main types of stroke: ischemic and hemorrhagic. In both cases the symptoms are the same, but treatments very different, so a cost-effective and portable classification device is needed.

In (Agnelli et al. 2020) a methodology for classifying stroke was proposed. The methodology combines the use of EIT data, the computation of VHED functions (Greenleaf et al. 2018) that have a geometric interpretation of the EIT data and finally machine learning applied to these VHED functions for the stroke classification. In this talk we continue this research line and extend the previous results to a more realistic scenario.

## [03129] Recent developments on integral equation approaches for Electrical Impedance Tomography

**Format :** Talk at Waseda University

**Author(s) :** Cristiana Sebu (University of Malta)

**Abstract :** The talk is focused on recent developments of reconstruction algorithms that can be used to approximate admittivity distributions in Electrical Impedance Tomography. The algorithms are non-iterative and are based on linearized integral equation formulations to allow reconstructions of the conductivity and/or permittivity distributions of two and three-dimensional domains from boundary measurements of both low and high-frequency alternating input currents and induced potentials. Reconstructions from noisy simulated data are obtained from single-time, time-difference and multiple-times data.

00471 (2/2) : 4D @D515 [Chair: Melody Alsaker]

## [04744] Monitoring of hemorrhagic stroke using Electrical Impedance Tomography

**Format :** Talk at Waseda University

**Author(s) :** Ville Kolehmainen (Department of Technical Physics, University of Eastern Finland)

**Abstract :** In this talk, we present recent progress in development of electrical impedance tomography (EIT) based bedside monitoring of hemorrhagic stroke. We present the practical setup and pipeline for this novel application of EIT and the image reconstruction method we have developed for it.

Feasibility of the approach is studied with simulated data from anatomically highly accurate simulation models and experimental phantom data from a laboratory setup

## [04874] Exploration of deep generative modelling approaches to electrical impedance tomography

**Format :** Talk at Waseda University

**Author(s) :** Valentina Candiani (University of Genoa)

**Abstract :** Reconstruction of conductivity images in electrical impedance tomography (EIT) requires the solution of a nonlinear inverse problem on noisy data. This problem is typically ill-conditioned and solution algorithms need either simplifying assumptions or regularization based on a priori knowledge.

In this work we study the applicability, the challenges and the limitations of some relatively new deep generative models such as score-based generative diffusion models and normalising flows, for both image reconstruction and medical anomaly detection. This talk will present some preliminary results obtained with such approaches in the application of EIT to the detection of stroke.

## [04904] Fast CGO-based absolute reconstructions for 3D EIT

**Format :** Talk at Waseda University

**Author(s) :** Peter Muller (Villanova University)Sarah Hamilton (Marquette University)

**Abstract :** Complex geometrical optics (CGO)-based methods for 3-D electrical impedance tomography are presented. Calderón's method and the  $t^{\exp}$  method are adapted for reconstructions from 3-D electrode data. These are the first absolute images to be produced from these methods for 3-D electrode data, both simulated and experimental. Some benefits of these CGO-based methods are that they provide real-time imaging and are shown to be robust to modelling errors such as electrode location and domain size.

## [05054] Use of reference measurements in electrical tomography

**Format :** Talk at Waseda University

**Author(s) :** Aku Seppänen (University of Eastern Finland )Laura E. Dalton (Duke University)Mikko Räsänen (University of Eastern Finland)Moe Pourghaz (North Carolina State University)

**Abstract :** Reconstruction methods in electrical resistance/capacitance tomography are often divided into classes of absolute and difference methods. While absolute reconstructions are based on data from a single time instant, difference reconstructions use reference data, to image the change of conductivity/permittivity from the reference state qualitatively. In this talk, we demonstrate that absolute reconstructions can also benefit from the use of reference data, when available, especially because it improves their tolerance to modeling errors.

# [00475] Variational methods and periodic solutions in the n-body problem

## Session Time & Room :

00475 (1/3) : 1C (Aug.21, 13:20-15:00) @E819

00475 (2/3) : 1D (Aug.21, 15:30-17:10) @E819

00475 (3/3) : 1E (Aug.21, 17:40-19:20) @E819

## Type : Proposal of Minisymposium

**Abstract :** The n-body dynamics have been studied by many prominent mathematicians and physicists for centuries. With the developments of mathematical and computational tools, there has been exciting progress during the past two decades. This progress includes variational approaches, stability, chaotic phenomenon, integrability, central configurations, solar system, space mission designs, and planetary formations, among many others. In this minisymposium, we aim to provide a forum for researchers to share the latest developments and exchange ideas.

## Organizer(s) : Mitsuru Shibayama

**Classification :** 70F10, 37D35, 70M20, 70G75

## Minisymposium Program :

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00475 (1/3) : 1C @E819 [Chair: Mitsuru Shibayama]

# [04108] Regularizing Fuel-Optimal, Multi-Impulse Trajectories with Second-Order Derivatives

## Format : Talk at Waseda University

**Author(s) :** Kenta Oshima (Hiroshima Institute of Technology)

**Abstract :** The present work implements analytical second-order derivatives for a direct multiple shooting-based regularized method of minimizing the fuel expenditure for spacecraft trajectories. The high-order dynamical information, such as the state transition tensor, expresses the Hessian matrix of the Lagrange function in the nonlinear programming problem. The result is an efficient tool for robustly and accurately computing fuel-optimal, multi-impulse trajectories in the regularized framework of removing singularities associated with null thrust impulses.

# [04642] Floquet Mode-Based Transfer between Halo Orbits Using Solar Sails

## Format : Talk at Waseda University

**Author(s) :** Toshihiro Chujo (Tokyo Institute of Technology)

**Abstract :** Transfer between halo orbits around the sun-Earth L2 using solar sails is discussed in the circular restricted three-body problem. The path planning and the corresponding tilting angle of the sail are determined based on the Floquet mode, such that the coefficient of the center manifold for transition to another family of the halo orbit is maximized while that of the unstable manifold is suppressed under a certain threshold.

# [04549] Low-energy Transfer to the Earth-Moon Periodic Orbit: CubeSat Application

## Format : Talk at Waseda University

**Author(s) :** Takuya Chikazawa (The University of Tokyo)

**Abstract :** This work investigates trajectories design for the ride-share spacecraft that begin with the Moon swing-by. In this type of trajectory design, mission designers need to consider uncertainties under limited propulsion capability. To aid trajectories design, established theory, such as manifold from periodic orbit in circular restricted three-body system, are often used. We demonstrate how to use such theory in actual mission design and operation phases.

# [04028] Transfer between Resonances via Lobe Dynamics in the Standard Map

## Format : Talk at Waseda University

**Author(s) :** Naoki Hiraiwa (Kyushu University)Isaia Nisoli (Universidade Federal do Rio de Janeiro)Yuzuru Sato (Hokkaido University)Mai Bando (Kyushu University)Shinji Hokamoto (Kyushu University)

**Abstract :** Lobe dynamics is a useful structure to reveal phase space transport of chaotic trajectories by stable and unstable manifolds of resonant orbits. Based on lobe dynamics, this study formulates the transfer problem between two quasi-periodic orbits to find the optimal lobe sequence. Especially, the lobe dynamics of resonant orbits of the standard map are extracted and used to solve the problem. Applications to spacecraft trajectory design are also discussed.

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00475 (2/3) : 1D @E819 [Chair: Guowei Yu]

## [03973] Distance estimates for action-minimizing solutions of the n-body problem

**Format :** Talk at Waseda University

**Author(s) :** Bo-Yu Pan (National Chung-Hsing University)

**Abstract :** In this talk we estimate mutual distances of action minimizing solutions for the n-body problem. We will present some quantitative estimates for these solutions, including their action values and bounds for their mutual distances. These estimates will facilitate numerical explorations to locate and search new orbits effectively.

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## [04970] Some progress on the N-center problem by variational methods

**Format :** Talk at Waseda University

**Author(s) :** Kuo-Chang Chen (National Tsing Hua University)

**Abstract :** Since Chenciner-Montgomery's construction of the figure-8 orbit for the 3-body problem, in the past 20+ years variational methods have succeeded in discovering new solutions for the N-body and N-center problems, within certain symmetry of topological classes. I will briefly outline recent progress, main ideas and obstacles, and some ongoing research topics for the N-center problem. In particular, I will outline variational construction of satellite orbits for N=2, and recent joint works with Guowei Yu on periodic and chaotic orbits for N>2.

## [04318] Periodic solutions bifurcated from the figure-eight choreography: non-planar eight and non-symmetric eight

**Format :** Talk at Waseda University

**Author(s) :** Hiroshi Fukuda (Kitasato University) Toshiaki Fujiwara (Kitasato University) Hiroshi Ozaki (Tokai University)

**Abstract :** The figure-eight choreography of equal mass three bodies under the homogeneous potential  $-1/r^\alpha$  and under the Lennard-Jones type potential  $1/r^{12} - 1/r^6$ , bifurcates in power  $\alpha$  and in period  $T$ , respectively, where  $r$  is a distance between bodies. We found two interesting bifurcation solutions: a figure-eight choreography with an orbit having no spatial symmetry, and a non-planar figure-eight solution which is unfortunately not choreographic.

## [04797] Variational structures for infinite transition orbits of monotone twist maps

**Format :** Talk at Waseda University

**Author(s) :** Yuika Kajihara (Kyoto university)

**Abstract :** There is a lot of study on the dynamics of area-preserving maps, and Poincare and Birkhoff's works are well-known. In this talk, we define a special class of area-preserving maps called monotone twist maps to consider the variational structures of area-preserving maps. Variational structures determined from twist maps can be used for constructing characteristic trajectories of twist maps. Our goal is to define the variational structure such as giving infinite transition orbits through minimizing methods.

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00475 (3/3) : 1E @E819 [Chair: Kuo-Chang Chen]

## [03812] Periodic and homo/heteroclinic solutions of the restricted three-body problem

**Format :** Talk at Waseda University

**Author(s) :** Mitsuru Shibayama (Kyoto University)

**Abstract :** The restricted three-body problem is an important research area that deals with significant issues in celestial mechanics, such as analyzing asteroid movement behavior and orbit design for space probes. We aim to show the existence of periodic and heteroclinic orbits in the planar circular R3BP. To find these orbits, we adopt a variational approach and symmetry.

**[04714] Existence of transit orbits in the restricted three-body problem****Format :** Talk at Waseda University**Author(s) :** Taiga Kurokawa (Kyoto University)Mitsuru Shibayama (Kyoto University)**Abstract :** We discuss the existence of transit orbits with fixed energy in the planar circular restricted three-body problem. In 2005, Moeckel provided sufficient conditions for the existence of transit orbits using the Maupertuis functional. In this talk, we give another sufficient condition using the Lagrange functional. This is joint work with Mitsuru Shibayama.**[03894] regularizable collinear periodic solutions in the n-body problem with arbitrary masses****Format :** Talk at Waseda University**Author(s) :** Guowei Yu (Nankai University)**Abstract :** For n-body problem with arbitrary positive masses, we prove there are regularizable collinear periodic solutions for any ordering of the masses, going from a simultaneous binary collision to another in half of a period with half of the masses moving monotonically to the right and the other half monotonically to the left. When the masses satisfy certain equality condition, the solutions have extra symmetry. This also gives a new proof of the Schubart orbit, when n=3.**[03430] Braids and periodic solutions of the planar N-body problem****Format :** Talk at Waseda University**Author(s) :** EIKO KIN (Osaka University)Yuika Kajihara (Kyoto University)Mitsuru Shibayama (Kyoto University)**Abstract :** Periodic solutions of the planar N-body problem determine braids through the trajectory of N bodies. Braids fall into three types: periodic, reducible and pseudo-Anosov. The last type is significant for the study of dynamical systems. In this talk I discuss a family of braid types obtained from periodic solutions, simple choreographies of the chain types by Guowei Yu and multiple choreographic solutions of the planar 2n-body problem by Shibayama.

# **[00479] Advances in clinically-driven AI image reconstruction and processing**

**Session Time & Room :** 1E (Aug.21, 17:40-19:20) @E818**Type :** Proposal of Minisymposium**Abstract :** The application of Artificial Intelligence methods, particularly in medical imaging, attracts huge interest from the mathematics and computer science community. Often, AI-based methods provide solutions surpassing image quality metrics compared to traditional methods. However, it's not always obvious if improved image quality metrics necessarily translate to improved clinically-relevant questions such as diagnosis and prognosis. This minisymposium focuses on applied AI methodologies that are clinically-oriented and incorporate direct measures and uses of clinical metrics in the learning or evaluation sections. We will cover topics including advances in model-based learned reconstruction, AI-based inverse problems, regularisation, generative models and their clinical applications.**Organizer(s) :** Ander Biguri, Lorena Escudero**Classification :** 68Txx, 92Cxx**Minisymposium Program :**

00479 (1/1) : 1E @E818 [Chair: Ander Biguri &amp; Lorena Escudero]

**[05254] The impact of model-based ML driven CT reconstruction on tumor segmentation and clinical diagnosis****Format :** Talk at Waseda University**Author(s) :** Ander Biguri (University of Cambridge)Carola-Bibiane Schönlieb (University of Cambridge)Lorena Escudero (University of Cambridge)**Abstract :** Machine learning has recently found success in tomographic image reconstruction, particularly CT. This work explores its impact on image quality, but most importantly, how (or if) that image quality translates to clinically relevant parameters, in this case radiomics. The evaluation of the reconstruction quality thus is moved from image quality metrics like SSIM or PSNR to clinically relevant metrics like predictive power of radiomics based tumour analysis.

## [03919] Bringing research advances in imaging sciences into the clinic

**Format :** Talk at Waseda University

**Author(s) :** Ozan Öktem (KTH Royal Institute of Technology)Lorena Escudero (University of Cambridge)Thomas Buddenotte (Jung Diagnostics GmbH)Cathal McCague (University of Cambridge)Carola-Bibiane Schönlieb (University of Cambridge)Evis Sala (University of Cambridge)

**Abstract :** The talk will survey both scientific and practical challenges associated with making state-of-the-art deep learning methods available to clinicians. It will showcase these challenges in an ambitious setting where one seeks to use an end-to-end deep learning based approach for joint reconstruction and downstream post-processing task, the latter being specific for a clinical use case.

## [02867] Spectral Normalisation of Depthwise Separable Convolutions for Medical Applications

**Format :** Talk at Waseda University

**Author(s) :** Christina Runkel (University of Cambridge)Christian Etmann (University of Cambridge)Michael Moeller (University of Siegen)Carola-Bibiane Schönlieb (University of Cambridge)

**Abstract :** An increasing number of models require the control of the spectral norm of convolutional layers of a neural network. While there is an abundance of methods for estimating and enforcing upper bounds on those during training, they are typically costly in either memory or time. In this talk, we introduce a very simple method for spectral normalisation of depthwise separable convolutions, which introduces negligible computational and memory overhead - allowing to control spectral norms for practical relevant applications like medical imaging.

## [05266] Mice PET/CT Dataset Augmentation using a 3D Single Image GAN

**Format :** Online Talk on Zoom

**Author(s) :** Jeremy Kim (Stanford University)Jonathan Fisher (Stanford University)Craig Levin (Stanford University)

**Abstract :** In this study, we applied GANs for 3D mice PET/CT data augmentation; these synthetic mice will be used in deep learning (DL) based preclinical research. The lack of available datasets makes it difficult for researchers to apply DL to solve tasks that involve small-animal datasets, such as emission-based attenuation correction for small-animals PET/MR. We applied the Single-Image GAN (SinGAN) Framework to generate multiple realistic synthetic PET/CT scans of mice from a limited number of examples.

# [00484] Matrix Analysis and Applications

**Session Time & Room :**

00484 (1/4) : 4C (Aug.24, 13:20-15:00) @G306

00484 (2/4) : 4D (Aug.24, 15:30-17:10) @G306

00484 (3/4) : 4E (Aug.24, 17:40-19:20) @G306

00484 (4/4) : 5B (Aug.25, 10:40-12:20) @G306

**Type :** Proposal of Minisymposium

**Abstract :** The goal of the minisymposium is to stimulate research and foster interaction of researchers. Its scope includes any topics in matrices and their applications. Matrix analysis is widely used in mathematics with applications in control and systems theory, image processing, operations research, scientific computing, statistics, and engineering. This minisymposium has multiple sessions which provide an opportunity for researchers to exchange ideas and recent developments in this active area of research. Participants are from Canada, China, Japan, Macau, Norway, Pakistan, Portugal, Singapore, South Korea, and USA.

**Organizer(s) :** Luyining Gan, Tin-Yau Tam, Qing-Wen Wang, Yang Zhang

**Classification :** 15AXX

**Minisymposium Program :**

00484 (1/4) : 4C @G306 [Chair: Tin-Yau Tam]

## [01267] Combinatorial Perron Parameters and Classes of Trees

**Format :** Talk at Waseda University

**Author(s) :** Enide Cascais Andrade (CIDMA, University of Aveiro, Portugal)Lorenzo Ciardo (University of Oxford)Geir Dahl (University of Oslo)

**Abstract :**

The main goal of this talk is to present recent results related with the combinatorial Perron parameters introduced in previous papers for certain classes of trees, and related bounds for these parameters. These parameters are related to algebraic connectivity of trees and corresponding centers.

## [01379] Poset matrices and associated algebras

**Format :** Talk at Waseda University

**Author(s) :** Gi-Sang Cheon (Sungkyunkwan University)

**Abstract :** We introduce the constructions of poset matrices by defining several partial compositions on the species of poset matrices. Some of these partial composition operations are shown to define a set operad structure. We also obtain various matrix algebras obtained from incidence algebras of Riordan posets.

## [01266] Majorization orders for $(0, \pm 1)$ -matrices

**Format :** Talk at Waseda University

**Author(s) :** Geir Dahl (University of Oslo)Alexander Guterman (Bar-Ilan University)Pavel Shteyner (Bar-Ilan University)

**Abstract :** Matrix majorization is a generalization of classical majorization for vectors; an important notion in many areas of mathematics. The talk gives some majorization background, and then presents a study of matrix majorization for  $(0, \pm 1)$ -matrices, i.e., matrices whose entries are restricted to 0, 1 and  $-1$ . In particular, we characterize when the zero vector is weakly majorized by a matrix, and discuss related results. Different connections are discussed, and characterizations of majorization are given.

## [00830] The ranks and decompositions of quaternion tensors

**Format :** Talk at Waseda University

**Author(s) :** Yang Zhang (University of Manitoba)Yungang Liang (University of Manitoba)

**Abstract :** Quaternion tensors have attracted more and more attentions in recent years. Many applications have been found in various areas. In this talk, we discuss the maximal ranks of quaternion tensors, in particular, the third-order case. We also investigate the canonical forms, CP and Tucker decompositions of some quaternion tensors.

00484 (2/4) : 4D @G306 [Chair: Yang Zhang]

## [03621] Log-majorization and inequalities of power means

**Format :** Talk at Waseda University

**Author(s) :** Sejong Kim (Chungbuk National University)

**Abstract :** As non-commutative versions of the quasi-arithmetic mean, we consider the Lim-Palfia's power mean, Renyi right mean, and Renyi power mean of positive definite matrices. We see that the Lim-Palfia's power mean of negative order converges increasingly to the log-Euclidean mean with respect to the weak log-majorization. Furthermore, we establish the weak log-majorization relationships between power means and provide the boundedness of Renyi power mean.

## [00868] Matrix Problems in International Economics

**Format :** Talk at Waseda University

**Author(s) :** Konstantin Kucheryavyy (University of Tokyo)

**Abstract :** Analyzing properties of general equilibrium models in economics amounts to analyzing properties of nonlinear systems of equations. The standard questions asked in this context are about existence and uniqueness of solutions to a nonlinear system of equations, characterization of multiplicity of solutions, and behavior of solutions in response to changes in parameters. One approach to address these questions is to formulate them in terms of matrix algebra. This approach has been especially fruitful when applied to classes of models arising in international economics. Such models often give rise to matrices with striking properties, but formally proving the observed properties usually

constitutes a challenge. In my presentation, I will consider several matrix problems that arise in the international economics context and sketch related proofs. I will also discuss open questions in this literature.

## [01404] Spectral inequalities for Kubo-Ando and Heinz means

**Format :** Talk at Waseda University

**Author(s) :** Rute Correia Lemos (CIDMA, University of Aveiro) Graça Soares (CMAT-UTAD, University of Trás-os Montes e Alto Douro)

**Abstract :** In this talk, spectral inequalities, involving Kubo-Ando operator connections and means of positive semidefinite matrices, are surveyed. Some Log-majorization type results are presented. Singular values inequalities for Heinz mean of matrices, which are not of Kubo-Ando type, and its 'harmonic' variant are also given.

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## [00800] Limit of the induced Aluthge transformations

**Format :** Talk at Waseda University

**Author(s) :** Takeaki Yamazaki (Toyo University)

**Abstract :** Let  $\mathcal{H}$  and  $B(\mathcal{H})$  be a complex Hilbert space and the algebra of all bounded linear operators on  $\mathcal{H}$ , respectively. For  $T \in B(\mathcal{H})$  with the polar decomposition  $T = U|T|$ , Aluthge transformation is known as  $\Delta(T) := |T|^{1/2}U|T|^{1/2}$ . In this talk, we shall introduce a generalization of Aluthge transformations and limit point of its iterations.

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00484 (3/4) : 4E @G306 [Chair: Sejong Kim]

## [01263] Geometric inequalities for contraction matrices

**Format :** Talk at Waseda University

**Author(s) :** Tin-Yau Tam (University of Nevada, Reno)

**Abstract :** Given two  $n \times n$  contraction matrices  $W$  and  $Z$ , i.e.,  $I - WW^* \geq 0$  and  $I - ZZ^* \geq 0$ , L.K. Hua's inequalities (1955) assert that

$$\det(I - WW^*) \det(I - ZZ^*) \leq |\det(I - WZ^*)|^2 \leq \det(I + WW^*) \det(I + ZZ^*). \quad (2)$$

In this talk we will present geometry behind Hua's inequalities in the context of elliptical and hyperbolic geometry.

## [01307] The generalized quaternion matrix equation

**Format :** Talk at Waseda University

**Author(s) :** Xin Liu (Macau University of Science and Technology) Cui E Yu (Macau University of Science and Technology)

**Abstract :** We consider the matrix equation  $AXB + CX^*D = E$  over the generalized quaternions, where  $X^*$  is one of  $X$ ,  $X^*$ , the  $\eta$ -conjugate or the  $\eta$ -conjugate transpose of  $X$  with  $\eta \in \{i, j, k\}$ . We define two new real representations of a generalized quaternion matrix, then we derive the solvability conditions for the mentioned matrix equation. Moreover, we also discuss the existence of  $X = \pm X^*$  solutions to the generalized quaternion matrix equation  $AXB + CXD = E$ .

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00484 (4/4) : 5B @G306 [Chair: Yang Zhang]

## [01222] Some new results on matrix and tensor equations

**Format :** Online Talk on Zoom

**Author(s) :** Qing-Wen Wang (Shanghai University, China)

**Abstract :** In this talk, we mainly introduce some new developments of matrix and tensor equations over the quaternion algebra.

## [01920] Matrix inequalities and properties of means on positive definite matrices

**Format :** Online Talk on Zoom

**Author(s) :** Luyining Gan (University of Nevada Reno)

**Abstract :** In this talk, we will introduce the study of the relations between the weighted metric geometric mean, the weighted spectral geometric mean and the weighted Wasserstein mean of the positive definite matrices in terms of

(weak) log-majorization relation. In addition, we will also introduce some new properties of means, like geodesic property and tolerance relation.

## [05621] How to check D-stability: a simple determinantal test

**Format :** Online Talk on Zoom

**Author(s) :** Volha Y. Kushel (Shanghai University)

**Abstract :** The concept of matrix  $D$ -stability, introduced in 1958 by Arrow and McManus is of major importance due to the variety of its applications. However, characterization of matrix  $D$ -stability for dimensions  $n > 4$  is considered as a hard open problem. In this talk, we propose a simple way for testing matrix  $D$ -stability, in terms of the inequalities between

principal minors of a matrix. The conditions are just sufficient but they allow to test matrices of an arbitrary size  $n$ , are easy to verify and can be used for the analysis of parameter-dependent models.

# [00488] Eigenvector-Dependent Nonlinear Eigenvalue Problems: Theory, Algorithms and Applications

**Session Time & Room :**

00488 (1/2) : 1E (Aug.21, 17:40-19:20) @E603

00488 (2/2) : 2C (Aug.22, 13:20-15:00) @E603

**Type :** Proposal of Minisymposium

**Abstract :** Nonlinear eigenvalue problems fall into two major categories in terms of eigenvalue-dependency or eigenvector-dependency, short-named NEP and NEPv, respectively. NEPv is the next natural topic after NEP. The most well-known origin of NEPv is from Kohn-Sham density functional theory in electronic structure calculations, but most recent sources are various machine learning models in the form of optimization on matrix manifolds, core-periphery detection in networks, rate-splitting multiple access in wireless communication, among others. In this minisymposium, speakers will present recent advancements in algorithms, numerical analysis and applications of NEPv and discuss emerging challenges.

**Organizer(s) :** Zhaojun Bai, Ren-Cang Li, Ding Lu

**Classification :** 65F15, 65H17, 90C25

**Minisymposium Program :**

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00488 (1/2) : 1E @E603 [Chair: Zhaojun Bai]

## [03905] A Self-Consistent-Field Iteration for OCCA

**Format :** Talk at Waseda University

**Author(s) :** Leihong Zhang (Soochow University) Li Wang (University of Texas at Arlington) Zhaojun Bai (University of California, Davis) Rencang Li (University of Texas at Arlington)

**Abstract :** In this talk, we propose an efficient algorithm for solving the orthogonal canonical correlation analysis (OCCA). Within an alternating optimization scheme, a customized self-consistent-field (SCF) iteration for a core trace-fractional sub-maximization over orthogonality constraint is devised and analyzed. The SCF iteration is further extended to deal with the multi-view OCCA. Experiments on real-world applications of multi-view learning will be reported.

## [04633] Mathematical Analysis and Numerical Approximations of Density Functional Theory Models for Metallic Systems

**Format :** Talk at Waseda University

**Author(s) :** Xiaoying Dai (Academy of Mathematics and Systems Science, Chinese Academy of Sciences)

**Abstract :** In this talk, we will introduce our study on the energy minimization model arising in the ensemble Kohn-Sham density functional theory for metallic systems, in which a pseudo-eigenvalue matrix and a general smearing approach are involved. We investigate the invariance of the energy functional and

the existence of the minimizer of the ensemble Kohn-Sham model. We propose an adaptive two-parameter step size strategy and the corresponding preconditioned conjugate gradient methods to solve the energy minimization model. Under some mild but reasonable assumptions, we prove the global convergence for the gradients of the energy functional produced by our algorithms. Numerical experiments show that our algorithms are efficient, especially for large scale metallic systems. In particular, our algorithms produce convergent numerical approximations for some metallic systems, for which the traditional self-consistent field iterations fail to converge. This is a joint work with Dr. Bin Yang and Prof. Aihui Zhou.

## [05119] Convergence of SCF Iteration for Eigenvector-dependent Nonlinear Eigenvalue Problems

**Format :** Talk at Waseda University

**Author(s) :** Ding Lu (University of Kentucky)

**Abstract :** The self-consistent field (SCF) iteration is a widely used method for solving eigenvector-dependent nonlinear eigenvalue problems (NEPv). Despite its simplicity, SCF is prone to slow convergence and can even fail to converge entirely. Extensive research has been devoted to analyzing the algorithm's convergence, and in this talk, we will share new insights on the local convergence analysis of SCF. First, for NEPv with a unitarily-invariant coefficient matrix, we will establish a precise estimation of the local convergence factor of SCF. This estimation enables us to prove the convergence of a level-shift scheme, which can help address the convergence issues of SCF. Second, for a class of NEPv without the unitary invariance property, we will show how to transform the problem into a unitarily invariant NEPv locally at the eigenbasis of interest. We will then establish the convergence rate of SCF based on this transformed problem. This work is a joint effort with Zhaojun Bai and Ren-Cang Li.

## [04225] Geometric inexact Newton method for generalized singular values

**Format :** Online Talk on Zoom

**Author(s) :** Weiwei Xu (Nanjing University of Information Science and Technology) Michael K. Ng (The University of Hong Kong) Zhengjian Bai (Xiamen University)

**Abstract :** We give new model formulations for computing arbitrary generalized singular value of a Grassmann matrix pair or a real matrix pair, where we need to solve matrix optimization problems with unitary constraints or orthogonal constraints. We propose a geometric inexact Newton-CG method for solving these optimization problems. Under some mild assumptions, we establish the global and quadratic convergence of the proposed method for the complex case. We illustrate its effectiveness by some numerical examples.

00488 (2/2) : 2C @E603 [Chair: Ding Lu]

## [05381] Nonlinear spectral graph theory: an overview of graph properties

**Format :** Online Talk on Zoom

**Author(s) :** Francesco Tudisco (Gran Sasso Science Institute) Dong Zhang (Peking University) Piero Deidda (Gran Sasso Science Institute)

**Abstract :** It is well-known that a variety of combinatorial graph quantities are approximated by the spectrum of relevant graph matrices, such as the Laplacian or the adjacency matrix. While very useful and widely used, these approximations are far from being tight. A generalization of the graph spectrum can be defined by considering nonlinear eigenvalue problems defined in terms of pairs of homogeneous convex functions. For quadratic functions, this definition boils down to the standard linear (matrix) eigenvalue problem. In this talk, we review several basic definitions and properties of nonlinear eigenproblems defined in terms of generic homogeneous pairs, and we then show how the corresponding eigenvalues can be used to provide tight approximations to fundamental graph quantities, including the multi-way Cheeger constant, the graph packing radius, the graph's max and min cuts, and graph's modularity.

## [05445] Solving Non-Convex Problems without Relaxation: Unexpected Usefulness of NEPv on Optimization Theory

**Format :** Online Talk on Zoom

**Author(s) :** Jeonghun Park (Yonsei University)

**Abstract :** Non-convex optimization problems arise in many applications of wireless communications and signal processing. To solve this, one typical principle is relaxing the original problem, obtaining a "convexified" solution, and repeat the process until convergence. In this talk, breaking away from this conventional approach, we develop an unorthodox method called spectral method. We also show that in some applications, this new approach offers significantly better performances with less complexity.

## [05390] Trace Minimization Principles on Matrix Manifolds

**Format :** Talk at Waseda University

**Author(s) :** Xin Liang (Tsinghua University)Ren-Cang Li (University of Texas at Arlington)Li Wang (University of Texas at Arlington)Leihong Zhang (Soochow University)

**Abstract :** This talk is concerned with establishing a trace minimization principle for two Hermitian matrix pairs: when is  $\inf_X \text{trace}(\widehat{A}X^HAX)$  subject to  $\widehat{B}X^HBX = I$  finite? Sufficient and necessary conditions are obtained and, when the infimum is finite, an explicit formula for it is presented in terms of the finite eigenvalues of the matrix pairs.

## [05272] Bound states in the continuum for a class of infinite matrices

**Format :** Talk at Waseda University

**Author(s) :** Ya Yan Lu (City University of Hong Kong)

**Abstract :** For certain infinite matrix  $A$ , the equation  $Ax = \lambda x$  may represent a boundary value problem (BVP) for  $\lambda$  in a real interval  $C$ . Such an equation models the scattering of incident waves by some objects. Without the incident waves,  $Ax = \lambda x$  is still an eigenvalue problem. A bound state in the continuum (BIC) is a special eigenpair with the eigenvalue  $\lambda \in C$ . In that case, the BVP for the same  $\lambda$  has no uniqueness. A nonlinear version is  $(A + D(x))x = \lambda x$ , where  $D(x)$  is a diagonal matrix with the  $(i, i)$  entry being  $d_i|x_i|^2$ . In this talk, we discuss linear and nonlinear BICs for a class of infinite matrices.

# [00496] Recent development in Quantum Simulation and Stochastic Methods

**Session Time & Room :**

00496 (1/3) : 3C (Aug.23, 13:20-15:00) @G704

00496 (2/3) : 3D (Aug.23, 15:30-17:10) @G704

00496 (3/3) : 3E (Aug.23, 17:40-19:20) @G704

**Type :** Proposal of Minisymposium

**Abstract :** This mini-symposium aims to bring together mathematicians and scientists working on quantum simulation and related topics to exchange ideas and share recent results. It highlights how the recent developments in computational tools, such as stochastic methods, quantum computing, fast algorithms, etc., make the simulation of large-scale or multiscale quantum systems feasible and thus expand the scope of quantum simulation. It also serves as a platform for presenting challenging quantum problems, which still call for novel methodologies to alleviate simulation costs.

**Organizer(s) :** Lihui Chai, Zhiwen Zhang, Zhennan Zhou

**Classification :** 35Q40, 81-08, 68Q12, 65C20

**Minisymposium Program :**

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00496 (1/3) : 3C @G704 [Chair: Zhiwen Zhang]

## [02786] Orthogonalization and Orthogonalization-free Algorithms

**Format :** Talk at Waseda University

**Author(s) :** Weiguo Gao (Fudan University)

**Abstract :** This talk consists of two parts. Orthogonalization algorithms are discussed in the first part. And we extend the error analysis result for shiftedCholeskyQR3 algorithm in oblique inner product and show that the new error bound is optimal. We also discuss the loss of orthogonality and verify our conclusions through numerical experiments. This is joint work with Rentao Xu. In the second part, orthogonalization-free algorithms are proposed to solve extreme eigenvalue problems. These algorithms achieve eigenvectors instead of eigenspace. Global convergence and local linear convergence are discussed. Efficiency of new algorithms are demonstrated on random matrices and matrices from computational chemistry. This is joint work with Yingzhou Li and Bichen Lu.

## [01872] Frozen Gaussian Sampling for mixed quantum-classical dynamics

**Format :** Talk at Waseda University

**Author(s) :** Zhennan Zhou (Peking University)Zhen Huang ( University of California, Berkeley)Limin Xu ( Tsinghua University)

**Abstract :** In this article, we propose a Frozen Gaussian Sampling (FGS) algorithm for simulating nonadiabatic quantum dynamics at metal surfaces with a continuous spectrum. This method consists of a Monte-Carlo algorithm for sampling the initial wave packets on the phase space and a surface-hopping type stochastic time propagation scheme for the wave packets. We prove that to reach a certain accuracy threshold, the sample size required is independent of both the semiclassical parameter and the number of metal orbitals, which makes it one of the most promising methods to study nonadiabatic dynamics. The algorithm and its convergence properties are also validated numerically. Furthermore, we carry out numerical experiments including exploring the nuclei dynamics, electron transfer, and finite-temperature effects, and demonstrate that our method captures the physics which can not be captured by classical surface hopping trajectories.

## [02280] The Random Feature Method for Time-dependent Problems

**Author(s) :** Jingrun Chen (University of Science and Technology of China)Weinan E (Peking University)Yixin Luo (Suzhou Institute for Advanced Research, University of Science and Technology of China)

**Abstract :** We propose to solve time-dependent partial differential equations in the framework of random feature method. The approximate solution is constructed using space-time partition of unity and random feature functions, and is proved to enjoy the universal approximation property. The resulting least-squares problem can be solved using two different strategies, and the corresponding error estimates are provided.

## [02728] Numerical methods for disordered NLS

**Format :** Talk at Waseda University

**Author(s) :** Xiaofei Zhao (Wuhan University)

**Abstract :** In this talk, I will consider the numerical solution for the disordered nonlinear Schrodinger equation (NLS). The model is a standard cubic NLS with a spatial random potential. The roughness and/or randomness of the potential brings some numerical difficulties. The performance of some classical time integrators will be reviewed, and the low-regularity integrator will be applied to tackle the possible roughness. Then, a quasi-Monte Carlo time-splitting method will be considered to tackle the randomness and improve the sampling accuracy. The full error bound will be presented and numerically verified.

00496 (2/3) : 3D @G704 [Chair: Zhennan Zhou]

## [02819] Asymmetric transport and topological invariants

**Format :** Talk at Waseda University

**Author(s) :** Guillaume Bal (University of Chicago)

**Abstract :** Transport asymmetries along interfaces separating insulating bulks have a topological origin. The talk proposes a classification of partial differential systems with topological invariant computed explicitly by a Fedosov-Hörmander formula. Asymmetric transport is associated to another topological invariant whose calculations is less direct. A bulk-edge correspondence states that the two invariants in fact agree. The theory is applied to graphene-based topological insulators. Time permitting, the above spectral analysis will be contrasted with a temporal picture.

## [02812] Asymmetric transport computations in Dirac models of topological insulators

**Format :** Talk at Waseda University

**Author(s) :** Zhongjian Wang (Nanyang Technological University)Guillaume Bal (University of Chicago)Jeremy Hoskins (University of Chicago)

**Abstract :** We will present a fast algorithm for computing transport properties of two-dimensional Dirac operators with linear domain walls, which model the macroscopic behavior of the robust and asymmetric transport observed at an interface separating two two-dimensional topological insulators. Our method is based on reformulating the partial differential equation as a corresponding volume integral equation, which we solve via a spectral discretization scheme. We demonstrate the accuracy of our method by confirming the quantization of an appropriate interface conductivity modeling transport asymmetry along the interface, and moreover, confirm that this quantity is immune to local perturbations. We also compute the far-field scattering matrix generated by such perturbations and verify that while asymmetric transport is topologically protected the absence of back-scattering is not.

## [01869] Quantum Orbital Minimization Method for Excited States Calculation on Quantum Computer

**Format :** Talk at Waseda University

**Author(s) :** Yingzhou Li (Fudan University)

**Abstract :** We propose a quantum-classical hybrid variational algorithm, the quantum orbital minimization method (qOMM), for obtaining the ground state and low-lying excited states of a Hermitian operator. Given parametrized ansatz circuits representing eigenstates, qOMM implements quantum circuits to represent the objective function in the orbital minimization method and adopts a classical optimizer to minimize the objective function with respect to the parameters in ansatz circuits. The objective function has an orthogonality constraint implicitly embedded, which allows qOMM to apply a different ansatz circuit to each input reference state. We carry out numerical simulations that seek to find excited states of H<sub>2</sub>, LiH, and a toy model consisting of four hydrogen atoms arranged in a square lattice in the STO3G basis with UCCSD ansatz circuits. Comparing the numerical results with existing excited states methods, qOMM is less prone to getting stuck in local minima and can achieve convergence with more shallow ansatz circuits.

## [02283] Bloch decomposition based method for Schroedinger equation with random inputs

**Format :** Talk at Waseda University

**Author(s) :** Zhongyi Huang (Tsinghua University)

**Abstract :** In this talk, we focus on the analysis and numerical methods for the Schroedinger equation with lattice potential and random inputs. Here we recall the well-known Bloch decomposition-based split-step pseudo-spectral method where we diagonalize the periodic part of the Hamilton operator so that the effects from dispersion and periodic lattice potential are computed together. Meanwhile, for the random non-periodic external potential, we utilize the generalize polynomial chaos with Galerkin procedure to form an ODE system which can be solved analytically. Furthermore, we analyse the convergence theory of the stochastic collocation method for the linear Schroedinger equation with random inputs. We provide sufficient conditions on the random potential and initial data to ensure the spectral convergence.

00496 (3/3) : 3E @G704 [Chair: Lihui Chai]

## [02028] On Quantum Speedups for Nonconvex Optimization via Quantum Tunneling Walks

**Format :** Online Talk on Zoom

**Author(s) :** Yizhou Liu (MIT)Weijie J. Su (University of Pennsylvania)Tongyang Li (Peking University)

**Abstract :** Classical algorithms are often not effective for solving nonconvex optimization problems where local minima are separated by high barriers. In this paper, we explore possible quantum speedups for nonconvex optimization by leveraging the global effect of quantum tunneling. Specifically, we introduce a quantum algorithm termed the quantum tunneling walk (QTW) and apply it to nonconvex problems where local minima are approximately global minima. We show that QTW achieves quantum speedup over classical stochastic gradient descents (SGD) when the barriers between different local minima are high but thin and the minima are flat. Based on this observation, we construct a specific double-well landscape, where classical algorithms cannot efficiently hit one target well knowing the other well but QTW can when given proper initial states near the known well. Finally, we corroborate our findings with numerical experiments.

## [02822] Quantum dynamics simulation and its application to Hamiltonian learning

**Format :** Online Talk on Zoom

**Author(s) :** Di Fang (Duke University)

**Abstract :** Recent years have witnessed tremendous progress in developing and analyzing quantum algorithms for quantum dynamics simulation (Hamiltonian simulation). The accuracy of quantum dynamics simulation is usually measured by the error of the unitary evolution operator in the operator norm, which in turn depends on the operator norm of the Hamiltonian. However, the operator norm measures the worst-case scenario, while practical simulation concerns the error with respect to a given initial vector or given observables at hand. In this talk, we will discuss a few ways to weaken the strong operator norm dependence in quantum simulation tasks by taking into account the the initial condition and observables. We then discuss how such analysis can be applied in the setting of Hamiltonian learning. Using a Hamiltonian reshaping technique, we propose a first learning algorithm to achieve the Heisenberg limit for efficiently learning an interacting N-qubit local Hamiltonian.

# [00497] Advances in numerical methods for nonlinear optics

**Session Time & Room :**

00497 (1/2) : 4D (Aug.24, 15:30-17:10) @D404

00497 (2/2) : 4E (Aug.24, 17:40-19:20) @D404

**Type :** Proposal of Minisymposium

**Abstract :** Nonlinear optics is the area of optics that studies the interaction of light with matter in the regime where the response of the material system to the applied electromagnetic field is nonlinear in the amplitude of this field. Here, we are concerned with numerical modeling of nonlinear optical phenomena. Of particular interest to this minisymposium are recent advances on general numerical methods such as finite difference methods, finite element methods, discontinuous Galerkin methods, etc. that have been tailored to the mathematical models of nonlinear optics with emphasis on achieving high order accuracy, adaptivity and efficient handling of multiscale features.

**Organizer(s) :** Vrushali A. Bokil, Camille Carvalho, Stéphane Lanteri, Claire Scheid

**Classification :** 78-10

**Minisymposium Program :**

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00497 (1/2) : 4D @D404 [Chair: Stéphane Lanteri]

## [03183] High-Order Accurate Approaches for Maxwell's Equations with Nonlinear Active Media on Overlapping Grids

**Format :** Talk at Waseda University

**Author(s) :** Jeffrey Banks (Rensselaer Polytechnic Institute)Gregor Kovacic (Rensselaer Polytechnic Institute)William Henshaw (Rensselaer Polytechnic Institute)Donald Schwendeman (Rensselaer Polytechnic Institute)Qing Xia (KTH Royal Institute of Technology)Alexander Kildeshev (Purdue University)Ludmila Prokopeva (Purdue University)

**Abstract :** Here I discuss efficient numerical methods for Maxwell's equations in nonlinear active media. Complex geometry is treated with overlapping grids, and interfaces between different materials are accurately and efficiently treated using compatibility coupling conditions. A novel hierarchical modified equation (ME) approach leads to an explicit scheme that does not require nonlinear iteration, and also gives local update equations without any tangential coupling along interfaces that would otherwise occur using a traditional high-order ME time stepper.

## [02203] Energy stability and active Q-factor control in numerical models of nonlinear electromagnetic resonance effects

**Format :** Online Talk on Zoom

**Author(s) :** Lutz Angermann (Clausthal University of Technology)

**Abstract :** The talk deals with the modeling and some properties of mathematical models to describe the excitation of a nonlinear material by electromagnetic waves, including typical questions such as the existence and uniqueness of a solution, the derivation of energy laws or estimates, the evaluation of the resonance quality and the transfer of these properties to numerical models.

## [02291] Energy stable finite element method for nonlinear Maxwell's equations

**Format :** Talk at Waseda University

**Author(s) :** Maohui Lyu (Beijing University of Posts and Telecommunications)Vrushali Bokil (Oregon State University)Yingda Cheng (Michigan State University)Fengyan Li (Rensselaer Polytechnic Institute)Weiyang Zheng (LSEC, Chinese academy of sciences)

**Abstract :** In this talk, we consider the time-domain nonlinear Maxwell's equations in multi-dimensions. With special discretizations for the nonlinear terms, we introduce a class of provably energy stable finite element method. Numerical experiments are provided to validate the performance of the proposed methods.

## [03742] High Order Energy Stable FDTD Methods for Maxwell Duffing models in Nonlinear Photonics

**Format :** Talk at Waseda University

**Author(s) :** Vrushali A Bokil (Oregon State University) Daniel Appelo (Michigan State University) Yingda Cheng (Michigan State University) Fengyan Li (Rensselaer Polytechnic Institute)

**Abstract :** We present electromagnetic models that describe nonlinear optical phenomenon in which the nonlinear polarization is driven by the electric field and modeled as an anharmonic oscillator(s). The models for the nonlinear polarization are given by Duffing equations and incorporate both nonlinearity and dispersion. Using the auxiliary differential equation approach, we present discretizations of the coupled Maxwell-Duffing models which are high order and energy stable methods based on finite difference time domain (FDTD) techniques.

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00497 (2/2) : 4E @D404 [Chair: Vrushali A Bokil]

## [05175] Local time-integration for wave equations

**Format :** Online Talk on Zoom

**Author(s) :** Constantin Carle (Karlsruhe Institute of Technology) Marlis Hochbruck (Karlsruhe Institute of Technology)

**Abstract :** For the spatially discretized acoustic wave equation, stability of explicit time integration schemes such as the leapfrog scheme can only be guaranteed under a CFL condition. In the case of locally refined meshes, this condition is the main bottleneck for the efficiency of explicit schemes.

To overcome this issue, we introduce local time-stepping and locally implicit schemes and present a rigorous error analysis.

## [02186] Discontinuous Galerkin Time-Domain methods for nonlinear active media on unstructured grids

**Format :** Talk at Waseda University

**Author(s) :** Stéphane Descombes (Université Côte d'Azur, CNRS, Inria, LJAD) Stéphane Lanteri (Université Côte d'Azur, Inria, CNRS, LJAD) Cédric Legrand (Université Côte d'Azur, Inria, CNRS, LJAD)

**Abstract :** We present a Discontinuous Galerkin Time-Domain method for solving the system of Maxwell equations coupled to the rate equations modeling light interaction with gain media.

## [00498] Approximation and modeling with manifold-valued data

**Session Time & Room :**

00498 (1/3) : 4C (Aug.24, 13:20-15:00) @A615

00498 (2/3) : 4D (Aug.24, 15:30-17:10) @A615

00498 (3/3) : 4E (Aug.24, 17:40-19:20) @A615

**Type :** Proposal of Minisymposium

**Abstract :** Application problems that involve data on differentiable manifolds are at the interface of numerical analysis and differential geometry. Researchers approach such tasks for various reasons: some make general efforts to transfer established methods from the Euclidean setting to nonlinear manifolds. Others are motivated by a specific application that requires one to work with manifold data.

This minisymposium aims at bringing together researchers working on approximation and modeling problems on Riemannian manifolds. A particular focus is on interpolation methods and applications in model reduction.

We aspire to create synergies and bridge the gap between different communities in this fascinating research field.

**Organizer(s) :** Nir Sharon, Ralf Zimmermann

**Classification :** 65Dxx, 41Axx, 53B50, Riemannian Computing, Model Reduction

**Minisymposium Program :**

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00498 (1/3) : 4C @A615 [Chair: Ralf Zimmermann]

part\_1

## [05470] Implicit integration along the low-rank manifold for stiff and nonlinear equations

**Format :** Online Talk on Zoom

**Author(s) :** Aaron Charous (MIT)Pierre F. J. Lermusiaux (MIT)

**Abstract :** We introduce a family of implicit integration methods for the dynamical low-rank approximation: the alternating-implicit dynamically orthogonal Runge-Kutta (ai-DORK) schemes. By alternating over the row and column space of the approximate solution, an efficient iterative low-rank linear solver is developed. To evaluate nonlinearities, we propose a local/piecewise polynomial approximation with adaptive clustering, and on-the-fly reclustering may be performed efficiently in the coefficient space. We demonstrate the proposed schemes on ill-conditioned, nonlinear, and realistic systems.

## [04268] Stochastic modeling of model uncertainties through Riemannian reduced-order representations

**Format :** Online Talk on Zoom

**Author(s) :** Hao Zhang (Duke University)Johann Guilleminot (Duke University)

**Abstract :** Molecular Dynamics (MD) simulations are widely used in computational materials science to explore the conformational space of atomistic systems, to analyze microscopic processes, and to evaluate macroscopic properties of interest. At the core of all MD simulations stands the selection of interatomic potentials, which can be calibrated by means of first-principles calculations or by solving inverse problems based on experimental observations. Such potentials are not uniquely defined in general, which raises the question of model uncertainties and their impact on MD-informed multiscale predictions. In this work, we propose a new probabilistic framework that enables the seamless integration of model-form uncertainties in atomistic computations. The approach relies on a stochastic reduced-order model involving a randomized Galerkin projection operator. An information-theoretic probabilistic model is specifically constructed on the tangent space to the manifold, taking advantage of Riemannian projection and retraction operators. We also explore statistical inference with a view toward inverse identification. We show, in particular, that the Fréchet mean can be constrained by solving a quadratic programming problem. Various applications are finally presented to demonstrate the relevance of the method, including toy examples in the Euclidean space and multiscale simulations on single layer graphene sheets. The proposed method offers key advantages, including a simple and interpretable low-dimensional parameterization, the ability to constraint the mean on the underlying manifold, and ease of implementation and propagation through multiscale operators.

## [05113] On approximation and representation of manifold-valued functions

**Format :** Talk at Waseda University

**Author(s) :** Nir Sharon (Tel Aviv University)

**Abstract :** Recent years have given rise to exciting developments in methods for approximating manifolds and manifold-valued objects. This talk will review recent work concerning manifold-valued approximation via refinement and quasi-interpolation operators and their close connection to multiscaling.

00498 (2/3) : 4D @A615 [Chair: Ralf Zimmermann]

## [05093] Multivariate Hermite Interpolation On Riemannian Manifolds

**Format :** Talk at Waseda University

**Author(s) :** Ralf Zimmermann (University of Southern Denmark)Ronny Bergmann (NTNU, Trondheim)

**Abstract :** We consider two methods for multivariate Hermite interpolation of manifold-valued functions.

On the one hand, we approach the problem via computing weighted Riemannian barycenters. This approach is intrinsic in the sense that it does not depend on local coordinates.

As an alternative, we consider straightforward Hermite interpolation in a tangent space. Here, the actual interpolation is conducted via classical vector space operations.

Both approaches are illustrated by means of numerical examples.

## [01628] Approximations and learning in the Wasserstein space

**Format :** Talk at Waseda University

**Author(s) :** Caroline Moosmueller (University of North Carolina at Chapel Hill)Alexander Cloninger (University of California, San Diego)Varun Khurana (University of California, San Diego)Harish Kannan (University of California, San Diego)Keaton Hamm (University of Texas at Arlington)

**Abstract :** Detecting differences and building classifiers between distributions, given only finite samples, are important tasks in a number of scientific fields. Optimal transport and the Wasserstein distance have evolved as the most natural concept in dealing with such tasks, but they also have some computational drawbacks.

In this talk, we describe an approximation framework through local linearizations that significantly reduces both the computational effort and the required training data in supervised learning settings.

## [05075] On multiscale quasi-interpolation of scattered scalar- and manifold-valued functions

**Format :** Talk at Waseda University

**Author(s) :** Nir Sharon (Tel Aviv University)Holger Wendland (University of Bayreuth)

**Abstract :** In this talk, we introduce and analyze a combination of kernel-based quasi-interpolation and multiscale approximations for both scalar- and manifold-valued functions. We are particularly interested in the improvements coming from such a combination over simply using quasi-interpolation processes alone. We provide ample numerical evidence that multiscale quasi-interpolation has superior convergence to quasi-interpolation. In addition, we will provide examples showing that the multiscale quasi-interpolation approach offers a powerful tool for data analysis tasks.

## [03824] The de Casteljau algorithm on symmetric spaces

**Format :** Online Talk on Zoom

**Author(s) :** Fátima Silva Leite (Institute of Systems and Robotics, University of Coimbra)Knut Huper (Institute of Mathematics, Julius-Maximilians-Universität Würzburg)

**Abstract :** An important task for interpolation problems in many areas of science and technology is the computation of smooth curves connecting two data points in a Riemannian symmetric space. For instance, the de Casteljau algorithm on manifolds, which is a geometric procedure to generate smooth polynomial splines, is based on recursive geodesic interpolation. Also in statistics, the efficient computation of (geometric) means of data in a symmetric space, as well as the computation of midpoints of smooth curves connecting two data points, is particularly important. While closed form solutions for the so called endpoint geodesic problem on general symmetric spaces are well known, often explicit exponentiation of matrices and/or SVD computations are still required. In most cases, these computations are rather expensive. We present much simpler closed form expressions for the particular case of Grassmannians, where only constant, linear and quadratic functions in the data points and scalar trigonometric functions are involved. This represents an important step in the implementation of the de Casteljau algorithm. We also comment on the general idea putting other important symmetric spaces, compact and noncompact ones, into perspective.

00498 (3/3) : 4E @A615 [Chair: Nir Sharon]

## [04608] Structure-preserving Model Order Reduction on Manifolds

**Format :** Talk at Waseda University

**Author(s) :** Patrick Buchfink (University of Stuttgart)Silke Glas (University of Twente)Bernard Haasdonk (University of Stuttgart)Benjamin Unger (University of Stuttgart)

**Abstract :** Approximation on manifolds has become a highly researched field in Model Order Reduction (MOR) for problems with slowly decaying Kolmogorov  $n$ -widths. However, many MOR techniques do not respect the structure of the underlying equations during the reduction.

In this talk, we present a new differential geometric formulation of MOR on pseudo-Riemannian manifolds. It allows us to geometrically understand and unify existing structure-preserving MOR techniques for Hamiltonian and Lagrangian systems.

## [03709] The Difference of Convex Algorithm on Riemannian Manifolds

**Format :** Online Talk on Zoom

**Author(s) :** Ronny Bergmann (NTNU, Trondheim)Orizon Pereira Ferreira (IME/UFG, Goiânia)Elisanderson Meneses Santos (Instituto Federal de Educação, Ciência e Tecnologia do Maranhão, Barra do Corda)João Carlos de Oliveira Souza (Department of Mathematics, Federal University of Piauí, Teresina)

**Abstract :** In this talk we propose a difference of convex algorithm (DCA) on Riemannian manifolds to solve optimisation problems involving a difference of two functions.

We establish both its relation to recently introduced Fenchel duality on manifolds, and its well-posedness. On Hadamard manifolds, we prove that every cluster point of the sequence generated by the algorithm is a cluster point.

Finally, we illustrate that several optimisation problems can be written as difference of convex (DC) functions on manifolds, and that some Euclidean problems that are differences of non-convex problems become DC problems when rephrased on a manifold. Numerical examples illustrate that such a rephrasing even for DC problems is beneficial numerically.

## [02950] Symplectic model order reduction via Riemannian optimization

**Format :** Talk at Waseda University

**Author(s) :** Bin Gao (Academy of Mathematics and Systems Science, Chinese Academy of Sciences)

**Abstract :** Numerous problems in optics, quantum physics, stability analysis, and control of dynamical systems can be brought to an optimization problem with matrix variable subjected to the symplecticity constraint. As this constraint nicely forms a so-called symplectic Stiefel manifold, Riemannian optimization is preferred, because one can borrow ideas from unconstrained optimization methods after preparing necessary geometric tools. Retraction is arguably the most important one which decides the way iterates are updated given a search direction. Two retractions have been constructed so far: one relies on the Cayley transform and the other is designed using quasi-geodesic curves. In this talk, we propose a new retraction that is based on an SR matrix decomposition. We prove that its domain contains the open unit ball which is essential in proving the global convergence of the associated gradient-based optimization algorithm. Moreover, we consider the symplectic model order reduction of Hamiltonian systems with various examples. The extensive numerical comparisons reveal the strengths of the proposed optimization algorithm.

## [05465] Hirotugu Akaike's Analysis of Gradient Descent: 70 years later

**Format :** Talk at Waseda University

**Author(s) :** Pok Yin Thomas Yu (Drexel University)

**Abstract :** It is very well known that when the exact line search gradient descent method is applied to a convex quadratic objective, the worst-case rate of convergence (among all seed vectors) deteriorates as the condition number of the Hessian of the objective grows.

By an elegant analysis by H. Akaike in 1959, it is generally believed -- but not proved -- that in the ill-conditioned regime the ROC for almost all initial vectors, and hence also the average ROC, is close to the worst case ROC. We complete Akaike's analysis using the theorem of center and stable manifolds. Our analysis also makes apparent the effect of an intermediate eigenvalue in the Hessian by establishing the following somewhat amusing result: In the absence of an intermediate eigenvalue, the average ROC gets arbitrarily fast -- not slow -- as the Hessian gets increasingly ill-conditioned.

We discuss in passing some contemporary applications of exact line search GD to polynomial optimization problems arising from imaging and data sciences and, if time allows, formulate an open problem related to accelerated GD methods.

## [00505] Structured matrices with applications in sciences and engineering

**Session Time & Room :**

00505 (1/3) : 5B (Aug.25, 10:40-12:20) @G305

00505 (2/3) : 5C (Aug.25, 13:20-15:00) @G305

00505 (3/3) : 5D (Aug.25, 15:30-17:10) @G305

**Type :** Proposal of Minisymposium

**Abstract :** The main purpose of this MS is to present recent developments on some special structured matrices that are of interest in different areas of mathematics, as well as in more applied areas like operations research, social sciences and computation. Problems arising in these fields are considered and techniques from matrix theory, numerical linear algebra and combinatorics, among others, are explored to solve them.

**Organizer(s) :** Susana Furtado, Natália Bebiano

**Classification :** 15A09, 15A29, 15B48, 47J20, 90B50

**Minisymposium Program :**

00505 (1/3) : 5B @G305 [Chair: Susana Furtado]

## [02264] Reciprocal Matrices, Ranking and the Relationship with Social Choice

**Format :** Online Talk on Zoom

**Author(s) :** Charles R Johnson (William and Mary)

**Abstract :** There is a close connection between the use of efficient vectors for reciprocal (pairwise comparison) matrices, used in business project ranking schemes, and social choice/voting rules from political science and economics. However,

the two seem not to have been discussed together before. We explore this connection, as well as advance the theory of reciprocal matrices. In addition, there seem to be natural connections with other parts of economic theory.

## [01723] A matrix approach to the study of efficient vectors in priority setting methodology

**Format :** Talk at Waseda University

**Author(s) :** Susana Furtado (Faculdade de Economia do Porto and CEAFL)Charles Johnson (College of William and Mary)

**Abstract :** The Analytic Hierarchy Process is a much discussed method in ranking business alternatives based on empirical and judgemental information.

Here we use a matrix approach to study the key component of efficient vectors for a reciprocal matrix of pairwise comparisons. In particular, we give new efficient vectors for a reciprocal matrix, which we compare numerically with other known efficient vectors.

## [00811] Singular matrices whose Moore-Penrose inverse is tridiagonal.

**Format :** Talk at Waseda University

**Author(s) :** Maria Isabel Bueno Cachadina (University of California Santa Barbara)Susana Borges Furtado (Faculdade de Economia do Porto and CEAFL)

**Abstract :** A variety of characterizations of nonsingular matrices whose inverse is tridiagonal (irreducible or not) have been widely investigated in the literature. One well-known such characterization is stated in terms of semiseparable matrices. In this talk, we consider singular matrices  $A$  and give necessary and sufficient conditions for the Moore-Penrose inverse of  $A$  to be tridiagonal. Our approach is based on bordering techniques, as given by Bapat and Zheng (2003). In addition, we obtain necessary conditions on  $A$  analogous to the semiseparability conditions in the nonsingular case, though in the singular case they are not sufficient, as illustrated with examples. We apply our results to give an explicit description of all the  $3 \times 3$  real singular matrices and  $3 \times 3$  Hermitian matrices whose Moore-Penrose inverse is irreducible and tridiagonal.

## [03060] Spectral geometric mean versus geometric mean by generalized Kantorovich constant

**Format :** Talk at Waseda University

**Author(s) :** Shigeru Furuichi (Nihon University)

**Abstract :** In this talk, we give two different operator inequalities between the weighted spectral geometric mean and the weighted geometric mean. We also study the mathematical properties for the generalized Kantorovich constant. Applying the obtained inequalities on the generalized Kantorovich constant, we give the ordering of two inequalities between the weighted spectral geometric mean and the weighted geometric mean.

In addition, we give some inequalities such as Ando type inequality, Kantorovich type inequality, and Ando-Hiai type inequality with the weighted spectral geometric mean and the generalized Kantorovich constant.

00505 (2/3) : 5C @G305 [Chair: Fernando Teran]

## [05539] Bundles of matrix pencils under strict equivalence

**Format :** Talk at Waseda University

**Author(s) :** FERNANDO DE TERÁN (Universidad Carlos III de Madrid)Froilán Martínez Dopico (Universidad Carlos III de Madrid)

**Abstract :** Bundles of matrix pencils are sets of pencils having the same Kronecker canonical form, up to the eigenvalues (namely, they are a union of orbits under strict equivalence). This notion was introduced in the 1990's, following the one for matrices under similarity (from Arnold, 1971). In this talk, we provide a characterization for the inclusion relation between closures of bundles and prove that bundles are open in their closure (in the standard topology).

## [05542] Row completion of polynomial matrices

**Format :** Talk at Waseda University

**Author(s) :** Alicia Roca (Universitat Politècnica de València / IMM, Valencia, Spain) Agurtzane Amparan (Universidad del País Vasco UPV/EHU) Itziar Baragaña (Universidad del País Vasco UPV/EHU) Silvia Marcaida (University of the Basque Country Universidad del País Vasco UPV/EHU)

**Abstract :** Perturbation problems arise frequently in applications, as in structural changes of the dynamics of a system or in pole placement problems in control theory.

Perturbation problems of matrices are closely related to completion problems. We present a solution to the row-completion problem of a polynomial matrix, prescribing the eigenstructure of the resulting matrix and maintaining the degree.

## [01819] Computational Techniques for the Mittag-Leffler Function of a Matrix Argument

**Format :** Talk at Waseda University

**Author(s) :** João R. Cardoso (Polytechnic Institute of Coimbra – ISEC)

**Abstract :** It is well-known that the two-parameter Mittag-Leffler function plays a key role in Fractional Calculus. In this talk, we address the problem of computing this function, when its argument is a square matrix. Effective methods for solving this problem involve the computation of successive derivatives or require the use of mixed precision arithmetic. We provide an alternative method that is derivative-free and can work entirely using IEEE standard double precision arithmetic. Our method starts with a reordered Schur decomposition of the argument matrix, so that the problem reduces to the computation of the Mittag-Leffler function of a triangular matrix with “close” eigenvalues. Theoretical and numerical issues regarding the performance of the method are investigated. A set of numerical experiments show that our novel approach is competitive with the existing ones, in terms of accuracy and computational cost.

## [02170] A reduction algorithm for reconstructing periodic pseudo-Jacobi matrices

**Format :** Online Talk on Zoom

**Author(s) :** Natalia Bebiano (Department of Mathematics, Coimbra University)

**Abstract :** For the given signature operator  $\mathcal{H} = I_r \oplus -I_{n-r}$ , a pseudo-Jacobi matrix is a self-adjoint matrix relatively to a symmetric bilinear form  $\langle \cdot, \cdot \rangle_{\mathcal{H}}$ . In this talk, we consider recent inverse eigenvalue problems for this class of matrices. Necessary and sufficient conditions under which the problems have solution are presented. Numerical algorithms are designed according to the obtained theoretical results. Illustrative numerical examples are given to test the reconstructive algorithms.

00505 (3/3) : 5D @G305 [Chair: Susana Furtado]

## [05469] A Low-Cost Algorithm to Determine Orbital Trajectories

**Format :** Talk at Waseda University

**Author(s) :** Sirani M. Perera (Embry-Riddle Aeronautical University) David Canales (Embry-Riddle Aeronautical University) Atahan Kurttisi (Embry-Riddle Aeronautical University) Brian Baker-McEvilly (Embry-Riddle Aeronautical University)

**Abstract :** The increasing demand for effective methods to propagate trajectories in the circular restricted three-body problem (CR3BP) is driven by heavy traffic in the region. This presentation introduces a novel approach that utilizes interpolation for determining orbital trajectories. We present a novel algorithm for determining orbital motion in the CR3BP, which is specifically applied to different Cislunar trajectories. Our findings demonstrate a 50% reduction in time complexity compared to the existing methods.

## [00506] Inverse Problems for Anomalous Diffusion

**Session Time & Room :**

00506 (1/3) : 3E (Aug.23, 17:40-19:20) @G808

00506 (2/3) : 4C (Aug.24, 13:20-15:00) @G808

00506 (3/3) : 4D (Aug.24, 15:30-17:10) @G808

**Type :** Proposal of Minisymposium

**Abstract :** Anomalous diffusion has received a lot of attention recently due to its extraordinary capability for describing nonstandard diffusion processes arising in multiple physical sciences and engineering. The relevant mathematical models often involve a fractional-order derivative in time or space. The nonlocality of the model substantially changes the analytical behaviour of the mathematical models when compared with the standard counterpart. This has also big impact on the behaviour of related inverse problems, which has witnessed many exciting and important developments in the last few years. In this mini-symposium, we aim at gathering researchers working on the topic to discuss recent advances on mathematical and numerical analysis of inverse problems for anomalous diffusion, in order to further promote the developments of the topic.

**Organizer(s) :** Bangti Jin, Zhi Zhou

**Classification :** 35R30, 35R11, 35B30

**Minisymposium Program :**

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00506 (1/3) : 3E @G808 [Chair: Bangti Jin]

### [01356] Coefficient identification space-fractional equation with Abel type operators

**Format :** Online Talk on Zoom

**Author(s) :** Barbara Kaltenbacher (University of Klagenfurt)

**Abstract :** We consider the inverse problem of recovering an unknown, spatially-dependent coefficient  $q(x)$  from the fractional order equation  $\mathbb{L}_\alpha u = f$  defined in a two-dimensional spatial domain from boundary information.

Here  $\mathbb{L}_\alpha = D_x^{\alpha_x} + D_y^{\alpha_y} + q(x)$  contains fractional derivative operators based on the Abel fractional integral.

We develop uniqueness and reconstruction results and show how the ill-conditioning of this inverse problem depends on the geometry of the region and the fractional powers  $\alpha_x$  and  $\alpha_y$ .

### [04481] Inverse problems for simultaneous determination of several scalar parameters and source factors in anomalous diffusion equations

**Format :** Online Talk on Zoom

**Author(s) :** Jaan Janno (Tallinn University of Technology)

**Abstract :** We consider inverse problems for anomalous diffusion equations where unknowns are orders of multiterm fractional time derivatives/multiterm fractional Laplacians or kernels of distributed fractional time derivatives/distributed fractional Laplacians. Along with these quantities an unknown is also a space-dependent or time-dependent source factor. We prove uniqueness for simultaneous determination of these quantities from final or boundary data.

### [03427] Parameter inverse problem for coupled time-fractional diffusion systems

**Format :** Talk at Waseda University

**Author(s) :** Yikan Liu (Hokkaido University)

**Abstract :** This talk is concerned with determining fractional orders in a coupled system of time-fractional diffusion equations. Defining the mild solution, we first establish fundamental unique existence of the solution, which mostly inherit those of a single equation. Owing to the coupling effect, we obtain the uniqueness for determining all orders by the single point observation of a single component of the solution.

### [04183] Identification of potential in diffusion equations from terminal observation

**Format :** Online Talk on Zoom

**Author(s) :** Zhidong Zhang (Sun Yat-sen University)

**Abstract :** We consider an inverse potential problem in a (sub)diffusion equation. We construct a monotone operator, one of whose fixed points is the unknown potential. The uniqueness of the identification is proved. Next, a fixed point iteration is applied to reconstruct the potential. We prove the linear convergence of the iterative algorithm and present a thorough error analysis for the reconstructed potential. Numerical experiments are provided to illustrate and complement our theoretical analysis.

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00506 (2/3) : 4C @G808 [Chair: Zhi Zhou]

## [04736] Classical Unique Continuation Property for Time Fractional Evolution Equations

**Format :** Talk at Waseda University

**Author(s) :** Gen Nakamura (Hokkaido University)Ching-Lung Lin (National Cheng Kung University)

**Abstract :** Let  $q_j = q_j(x)$ ,  $2 \leq j \leq m$  with  $q_1 = 1$  and let  $2 > \alpha = \alpha_1 > \alpha_2 > \dots > \alpha_m > 0$ .

Then, the classical unique continuation property of solutions in  $H^{\alpha,2}((0,T) \times \Omega)$  holds for the time fractional evolution equation (tfEE) whose leading part given as

$\sum_{j=1}^m q_j \partial_t^{\alpha_j} u(t, y) - L u(t, y)$  over a domain  $\Omega \subset \mathbb{R}^n$

with a time dependent strongly elliptic operator  $L$  of oder 2, where  $\partial_t^{\alpha_j}$  is the Caputo derivative whenever  $\alpha_j \notin \mathbb{Z}$ .

See C-L. Lin and G. Nakamura, Math. Ann. 385 (2023), pp. 551–574 for the details.

## [02704] The Calderón problem for nonlocal parabolic operators

**Format :** Talk at Waseda University

**Author(s) :** Yi-Hsuan Lin (Department of Applied Mathematics, National Yang Ming Chiao Tung University)

**Abstract :** We investigate inverse problems in the determination of leading coefficients for nonlocal parabolic operators, by knowing the corresponding Cauchy data in the exterior space-time domain. The key contribution is that we reduce nonlocal parabolic inverse problems to the corresponding local inverse problems with the lateral boundary Cauchy data. In addition, we derive a new equation and offer a novel proof of the unique continuation property for this new equation. We also build both uniqueness and non-uniqueness results for both nonlocal isotropic and anisotropic parabolic Calderón problems, respectively.

## [02699] Inverse Problems for Subdiffusion from Observation at an Unknown Terminal Time

**Format :** Talk at Waseda University

**Author(s) :** Bangti Jin (The Chinese University of Hong Kong)Yavar Kian (Aix Marseille University)Zhi Zhou (The Hong Kong Polytechnic University)

**Abstract :** Time-fractional subdiffusion equations represent an important class of mathematical models with a broad range of applications. The related inverse problems of recovering space-dependent parameters, e.g., initial condition, space dependent source or potential coefficient, from the terminal observation have been extensively studied in recent years. However, all existing studies have assumed that the terminal time at which one takes the observation is exactly known. In this talk, we present uniqueness and stability results for three canonical inverse problems, e.g., backward problem, inverse source and inverse potential problems, from the terminal observation at an unknown time. The subdiffusive nature of the problem indicates that one can simultaneously determine the terminal time and space-dependent parameter.

## [04403] Numerical Recovery of Multiple Parameters from One Lateral Boundary Measurement

**Format :** Talk at Waseda University

**Author(s) :** Siyu Cen (The Hong Kong Polytechnic University)Bangti Jin (Chinese University of Hong Kong)Yikan Liu (Hokkaido University)Zhi Zhou (The Hong Kong Polytechnic University)

**Abstract :** This talk is concerned with numerically recovering multiple parameters in a partly unknown subdiffusion model from one lateral measurement on the boundary. We prove that the boundary measurement uniquely determines the fractional order and the polygonal support of the diffusion coefficient, without knowing either the initial condition or the source. We present an algorithm for recovering the fractional order and diffusion coefficient which combines small-time asymptotic expansion, analytic continuation and the level set method.

00506 (3/3) : 4D @G808 [Chair: Yikan Liu]

## [04435] Long-Short time asymptotic estimates for time-fractional diffusion-wave equation

**Format :** Talk at Waseda University

**Author(s) :** Xinchi HUANG (Tokyo Institute of Technology)Xinchi Huang (Tokyo Institute of Technology)Yikan Liu (Hokkaido University)

**Abstract :** In this talk, we consider the time-fractional diffusion-wave equations and show the long-time asymptotic estimate of the solution, which can be used to prove the long-time strict positivity of the solution and the uniqueness for

an inverse source problem of determining the time-varying factor. Besides, we discuss the short-time asymptotic behavior and provide an application to the determination of the spatial varying factor in the source.

## [04612] Numerical identification of conductivity in (sub)diffusion equations from terminal measurement

**Format :** Online Talk on Zoom

**Author(s) :** Bangti Jin (Chinese University of Hong Kong)Xiliang Lu (Wuhan University)Qimeng Quan (Wuhan University)Zhi Zhou (The Hong Kong Polytechnic University)

**Abstract :** This talk focuses on the inverse diffusion problems in (sub)diffusion equation. Typically, we employ Tikhonov strategy and discretize the regularized model by finite element methods. One critical issue is to establish a priori error estimate on the concerned parameter. In this talk, the speaker will discuss their recent study of recovering a space-dependent diffusion coefficient from terminal observation by a novel conditional stability.

## [00507] Stochastic Dynamical Systems and Applications

**Session Time & Room :**

00507 (1/4) : 3D (Aug.23, 15:30-17:10) @G802

00507 (2/4) : 3E (Aug.23, 17:40-19:20) @G802

00507 (3/4) : 4C (Aug.24, 13:20-15:00) @G802

00507 (4/4) : 4D (Aug.24, 15:30-17:10) @G802

**Type :** Proposal of Minisymposium

**Abstract :** The objective of this special minisymposium is to bring together experts from multiple disciplines with complementary views and approaches to stochastic dynamics in the context of applications. The topics include but not limited to: Theoretical advances in stochastic dynamical systems and stochastic partial differential equations, connection with non-equilibrium statistical physics, non-Gaussian noise and nonlocal partial differential operators, dynamical indicators for phase transition and abrupt change, most probable transition pathways and early warning time, tools for predicting rare events or extreme events, machine learning tools for examining stochastic dynamics, multi-scale stochastic simulation algorithms, multiscale multiphase flow simulation and homogenization problems.

**Organizer(s) :** Yanjie Zhang

**Classification :** 37A50, 35R60, 60H17

**Minisymposium Program :**

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00507 (1/4) : 3D @G802

## [04264] Three-dimensional numerical study on wrinkling of vesicles in elongation flow

**Format :** Talk at Waseda University

**Author(s) :** Wang Xiao (Huazhong University of Science and Technology)

**Abstract :** We study the wrinkling dynamics of three-dimensional vesicles in time-dependent elongation flow by utilizing an immersed boundary method. The numerical results well match the predictions of perturbation analysis for a quasi-spherical vesicle. The parallel simulation can compute  $512^3$  Eulerian fluid grids and save the computation cost by at least an order of magnitude compared with the CPU algorithm. In addition, the parallel simulation can be directly extended to study other initial vesicles and external flows.

## [04452] Energetic Variation associated with nonlinear Schrödinger equations with Anderson Hamiltonian

**Format :** Talk at Waseda University

**Author(s) :** Qi Zhang (Yau Mathematical Sciences Center, Tsinghua University, China/Yanqi Lake Beijing Institute of Mathematical Sciences and Applications, China)

**Abstract :** We study the variation problem associated with nonlinear Schrödinger equations with Anderson Hamiltonian in 2-dimensional torus. Under the paracontrolled distribution framework from singular SPDEs theory, we obtain the existence of the ground state solution by considering the minimization problem of the corresponding energy functional

with  $L^2$  constraints. We also obtain the tail estimate on the distribution of the principal eigenvalue via the variational representation. This is joint work with Prof. Jinqiao Duan.

## [04457] Macroscopic approximation for stochastic N-particle system with small mass

**Format :** Talk at Waseda University

**Author(s) :** Wei Wang (Nanjing University)

**Abstract :** In this talk we present a small mass limit approximation on macroscopic scale for stochastic  $N$ -particle system.

On macroscopic scale we have a slow-fast system and then by coupling the system on microscopic scale, an averaging approach is applied to derive the small mass limit. We also present this method to several different systems.

## [04557] Effective wave factorization for a stochastic Schrodinger equation

**Format :** Talk at Waseda University

**Author(s) :** Ao Zhang (Central South University)

**Abstract :** We study the homogenization of a stochastic Schrodinger equation with a large periodic potential in solid state physics. Under a generic assumption on the spectral properties of the associated cell problem, we prove that the solution can be approximately factorized as the product of a fast oscillating cell eigenfunction and of a slowly varying solution of an effective equation. Our method is based on two-scale convergence and Bloch waves theory.

00507 (2/4) : 3E @G802

## [04528] Approximation of nonlinear filtering for multiscale McKean-Vlasov stochastic differential equations

**Format :** Talk at Waseda University

**Author(s) :** Huijie Qiao (Southeast University) Wanlin Wei (Southeast University)

**Abstract :** The work concerns approximation of nonlinear filtering for multiscale McKean-Vlasov stochastic differential equations. First of all, by a Poisson equation we prove an average principle. Then we define nonlinear filtering of the origin multiscale equations and the average equation, and again by the Poisson equation show approximation between nonlinear filtering of the slow part for the origin multiscale equations and that of the average equation.

## [04629] On the WKB approximation of confluent hypergeometric systems

**Format :** Talk at Waseda University

**Author(s) :** Xiaomeng Xu

**Abstract :** This talk studies the WKB approximation of the linear meromorphic systems of Poncaré rank 1 via the isomonodromy approach. It gives a characterization of the WKB approximation via the periods on the underlying spectral curves. It also unveils a relation between the WKB approximation, the Cauchy interlacing inequality, cluster algebras and so on. It is based on a joint work with Anton Alekseev, Andrew Neitzke and Yan Zhou.

## [04570] Global stability of stochastic functional differential equations

**Format :** Talk at Waseda University

**Author(s) :** Xiang Lyu (Shanghai Normal University)

**Abstract :** This paper gives a criterion for the existence of a stationary solution for a class of semilinear stochastic functional differential equations with additive white noise and its global stability. To be more precise, we show that the infinite-dimensional stochastic flow possesses a unique globally attracting random equilibrium in the state space of continuous functions, which produces the globally stable stationary solution.

## [04648] Averaging principle for slow-fast systems of stochastic PDEs with rough coefficients

**Format :** Online Talk on Zoom

**Author(s) :** Yichun Zhu (University of Maryland, College Park) Sandra Cerrai (University of Maryland, College Park)

**Abstract :** In this paper, we consider a class of slow-fast systems of stochastic partial differential equations where the nonlinearity in the slow equation is not continuous and unbounded.

We first provide conditions that ensure the existence of a martingale solution. Then we prove that the laws of the slow motions are tight, and any of their limiting points is a martingale solution for a suitable averaged equation. Our results apply to systems of

stochastic reaction-diffusion equations where the reaction term in the slow equation is only continuous and has polynomial growth.

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00507 (3/4) : 4C @G802

## [04756] Mean Asymptotic Behavior for Stochastic Kuramoto-Sivashinsky Equation in Bochner Spaces

**Format :** Online Talk on Zoom

**Author(s) :** Xiaopeng Chen (Shantou University)

**Abstract :** In this talk we mainly present some asymptotic behavior of the Kuramoto-Sivashinsky equation with stochastic perturbation. We define the mean random dynamical systems for the stochastic Kuramoto-Sivashinsky equation in Bochner spaces. Then we consider the so-called weak pullback mean random attractor and invariant manifold for the stochastic Kuramoto-Sivashinsky equation with odd initial conditions.

## [04325] The Poisson Equation and Application to Multi-Scale SDEs with State-Dependent Switching

**Format :** Online Talk on Zoom

**Author(s) :** Xiaobin Sun (Jiangsu Normal University)

**Abstract :** In this talk, we discuss the Poisson equation associated with a Markov chain. By investigating the differentiability of the corresponding transition probability matrix with respect to parameters, we establish the regularity of the Poisson equation solution. As an application, we further study the averaging principle for a class of multi-scale stochastic differential equations with state-dependent switching, ultimately achieving an optimal strong convergence order of 1/2. This talk is based on a joint work with Yingchao Xie.

## [04954] A stochastic fractional Schrodinger equation with multiplicative noise

**Format :** Talk at Waseda University

**Author(s) :** Yan jie Zhang (Zhengzhou University)Yanjie Zhang (Zhengzhou University )

**Abstract :** We establish the stochastic Strichartz estimate for the fractional Schrödinger equation with multiplicative noise. With the help of the deterministic Strichartz estimates, we prove the existence and uniqueness of a global solution to the stochastic fractional nonlinear Schrödinger equation in  $L_2(\mathbb{R}^n)$  and  $H^1(\mathbb{R}^n)$ , respectively. In addition, we also prove a general blow up result by deriving a localized virial estimate and the generalized Strauss inequality with  $E[u_0] < 0$ .

## [05083] The most probable dynamics of receptor-ligand binding on cell membrane

**Format :** Online Talk on Zoom

**Author(s) :** Xi Chen (Xi'an University of Finance and Economics)

**Abstract :** We devise a method for predicting receptor-ligand binding behaviors, based on stochastic dynamical modelling. We consider the receptor and ligand perform different motions and are thus modeled by stochastic differential equations with Gaussian noise or non-Gaussian noise. We use neural networks based on Onsager-Machlup function to compute the probability of the receptor diffusing to the cell membrane. In this way, we conclude with some indication about where the ligand will most probably encounter the receptor.

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00507 (4/4) : 4D @G802

## [00509] Recent developments in stochastic optimization

**Session Time & Room :**

00509 (1/2) : 3E (Aug.23, 17:40-19:20) @A201

00509 (2/2) : 4C (Aug.24, 13:20-15:00) @A201

**Type :** Proposal of Minisymposium

**Abstract :** Optimization problems involving stochastic models or randomized algorithms are at the core of various applications areas such as machine learning, finance, energy production, signal processing, telecommunications, and medical imaging. Modern applications involve complex models and large dimensions. They require sophisticated analysis and algorithmic tools to obtain efficiently reliable solutions. This minisymposium will feature several advances illustrating the fertile interface between stochastic analysis and optimization through talks presented by junior and senior researchers. It will cover theoretical advances, as well as practical applications in finance, optimal control, inverse problems, optimal transportation, and petroleum production.

**Organizer(s) :** Patrick L. Combettes

**Classification :** 90C15, 90C30, 46N10, 90C48

**Minisymposium Program :**

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00509 (1/2) : 3E @A201 [Chair: Patrick Combettes]

## [00650] Random activations in primal-dual splittings for monotone inclusions with a priori information

**Format :** Talk at Waseda University

**Author(s) :** Luis Briceño-Arias (Universidad Técnica Federico Santa María)

**Abstract :** In this paper, we propose a numerical approach for solving composite primal-dual monotone inclusions with a priori information. The underlying a priori information set is represented by the intersection of fixed point sets of a finite number of operators, and we propose an algorithm that activates the corresponding set by following a finite-valued random variable at each iteration. Our formulation is flexible and includes, for instance, deterministic and Bernoulli activations over cyclic schemes, and Kaczmarz-type random activations. The almost sure convergence of the algorithm is obtained by means of properties of stochastic Quasi-Fejér sequences. We also recover several primal-dual algorithms for monotone inclusions without a priori information and classical algorithms for solving convex feasibility problems and linear systems. In the context of convex optimization with inequality constraints, any selection of the constraints defines the a priori information set, in which case the operators involved are simply projections onto half spaces. By incorporating random projections onto a selection of the constraints to classical primal-dual schemes, we obtain faster algorithms as we illustrate by means of a numerical application to a stochastic arc capacity expansion problem in a transport network.

## [01376] New results on Carathéodory integral functions, applications to stochastic optimization

**Format :** Talk at Waseda University

**Author(s) :** Minh Nhut Bui (Universität Graz)Patrick L. Combettes (North Carolina State University)

**Abstract :** We present new results on Carathéodory integral functions and discuss applications to stochastic optimization.

## [03790] Adaptive partition-based method for 2-stage stochastic linear programming

**Format :** Talk at Waseda University

**Author(s) :** Eduardo Moreno (Universidad Adolfo Ibañez)Ivana Ljubic (ESSEC Business School)

**Abstract :** The Generalized Adaptive partition-based method for solving 2-stage stochastic linear problems is based on iteratively and automatically aggregating the uncertainty space into scenarios and disaggregating them based on the dual subproblem variables. It can be seen as a Benders-like method, where optimality cuts are adaptively aggregated based on the dual solutions. Computational experiments show significant improvements compared to classical methods, including the possibility of solving problems in continuous probability spaces using discrete optimization.

## [03978] Multistage optimization of a partially observed petroleum production system

**Format :** Talk at Waseda University

**Author(s) :** Jean-Philippe Chancelier (CERMICS -- Ecole des Ponts ParisTech)Pierre Carpentier (UMA, ENSTA PARIS)Michel De Lara (CERMICS - Ecole des Ponts ParisTech)Cyrille Vessaire (CERMICS -- Ecole des Ponts ParisTech)Alejandro Rodriguez-Martinez (Total Energies, SE Pau)

**Abstract :** An oil production network is composed of one or more reservoirs (geological formations containing oil) connected through a network of wells and pipes. At the beginning of the reservoir exploitation, we have only partial knowledge of the content of the reservoir, namely a probability distribution of the initial state of the reservoir.

We propose a formulation of the management of an oil production network where the reservoir is a partially observed controlled dynamical system. This approach leads to a well-known class of problems: Partially Observed Markovian Decision Process (POMDP). However, general POMDPs are often untractable due to the curse of dimensionality. In the case of the proposed formulation, we consider a subclass of POMDPs: deterministic-POMDPs (deterministic transition and observation). We highlight and exploit structure in the deterministic-POMDP formulation to push back the curse of dimensionality. Then, we are able to use Dynamic Programming to find the optimal production planning.

Finally, we present numerical applications.

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00509 (2/2) : 4C @A201 [Chair: Patrick Combettes]

## [05112] Convex stochastic optimization

**Format :** Talk at Waseda University

**Author(s) :** Teemu August Pennanen (King's College London)Ari-Pekka Perkkiö (Ludwig-Maximilian University of Munich)

**Abstract :** We study dynamic programming, duality and optimality conditions in general convex stochastic optimization problems introduced by Rockafellar and Wets in the 70s. We give a general formulation of the dynamic programming recursion and derive an explicit dual problem in terms of two dual variables, one of which is the shadow price of information while the other one gives the marginal cost of a perturbation much like in classical Lagrangian duality. Existence of primal solutions and the absence of duality gap are obtained without compactness or boundedness assumptions. In the context of financial mathematics, the relaxed assumptions are satisfied under the well-known no-arbitrage condition and the reasonable asymptotic elasticity condition of the utility function. We extend classical portfolio optimization duality theory to problems of optimal semi-static hedging. Besides financial mathematics, we obtain several new results in stochastic programming and stochastic optimal control.

## [00517] Numerical Modelling of Highly Flexible Structures for Industrial Applications

**Session Time & Room :** 3C (Aug.23, 13:20-15:00) @E606

**Type :** Proposal of Minisymposium

**Abstract :** Highly flexible slender structures like yarns, cables, hoses or ropes are essential parts of high-performance engineering systems. The complex response of such structures in real operational conditions is far beyond the capabilities of current modelling tools that are at the core of modern product development cycles. The European Training Network THREAD, see <https://thread-etn.eu/>, addresses this problem class by novel methods for modelling and numerical simulation and their application in medical engineering, ropeway system design, civil engineering and automotive industry. Three groups of the THREAD network report on modelling aspects and tailored geometric time integration methods in these fields of application.

**Organizer(s) :** Martin Arnold, Sigrid Leyendecker, Dejan Zupan

**Classification :** 65Lxx, 65P10, 37M15, 34A26

**Minisymposium Program :**

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00517 (1/1) : 3C @E606 [Chair: Martin Arnold]

## [02070] Augmented Lagrangian contact formulation of the 2D Euler elastica

**Format :** Talk at Waseda University

**Author(s) :** Martina Stavole (Friedrich-Alexander-Universität Erlangen-Nürnberg)Rodrigo Takuro Sato Martín de Almagro (Friedrich-Alexander-Universität Erlangen-Nürnberg)Olivier Brüls (Université de Liège )Sigrid Leyendecker (Friedrich-Alexander-Universität Erlangen-Nürnberg)

**Abstract :** In this work we show an application of an augmented Lagrangian formulation to simulate contact between an elastic curve and a narrow environment with rigid walls. Our goal is to provide fast and accurate simulations of endoscopic procedures.

## [02324] The velocity-based formulation for static and dynamic analysis of non-linear three-dimensional frames

**Format :** Talk at Waseda University

**Author(s) :** Dejan Zupan Sudhanva Kusuma Chandrashekara (University of Ljubljana)Eva Zupan (University of Ljubljana)

**Abstract :** The choice of primary interpolated variables is highly important in numerical formulations of three-dimensional frame-like structures. The crucial idea exploited in our approach is to employ velocities and angular velocities as the primary unknowns, which enables us the use of standard additive interpolation without violating the properties of configuration space. The main advantage of the proposed solution method is in its simplicity, robustness and long-term stability.

## [02419] Half-explicit time integration of constrained mechanical systems on Lie groups

**Format :** Online Talk on Zoom

**Author(s) :** Martin Arnold (Martin Luther University Halle-Wittenberg)

**Abstract :**

Recently, there has been new interest in the local coordinates approach to Lie group time integration. The present paper contributes a novel half-explicit Lie group integrator to this field of research. This half-explicit integrator combines an explicit Runge-Kutta Munthe-Kaas method with the index-2 formulation of the equations of motion for constrained mechanical systems. We construct methods of order up to  $p = 5$  and illustrate their favourable properties by numerical test results.

## [02155] Frequency-dependent damping as forcing on multisymplectic integrators

**Format :** Online Talk on Zoom

**Author(s) :** Rodrigo Takuro Sato Martín de Almagro (FAU - Lehrstuhl für Technische Dynamik)Sigrid Leyendecker (FAU - Lehrstuhl für Technische Dynamik)

**Abstract :** Multisymplectic integrators are geometric integration methods with interesting conservation properties. However, for the temporal integration of flexible structures it may be desirable to dampen high-frequency modes. In this talk we propose a simple frequency-dependent damping model which can be considered as additional forcing. We implement it together with multisymplectic integrators and compare its performance with the generalized alpha method, a popular numerical method for this application due to its frequency-dependent numerical damping.

# [00521] Recent advances on non-convex optimization in inverse problems, imaging and machine learning

**Session Time & Room :**

00521 (1/5) : 3D (Aug.23, 15:30-17:10) @A206

00521 (2/5) : 3E (Aug.23, 17:40-19:20) @A206

00521 (3/5) : 4C (Aug.24, 13:20-15:00) @A206

00521 (4/5) : 4D (Aug.24, 15:30-17:10) @A206

00521 (5/5) : 4E (Aug.24, 17:40-19:20) @A206

**Type :** Proposal of Minisymposium

**Abstract :** Non-convex optimization has become increasingly important for modern data science applications, with many unsolved challenging open problems. Due to the absence of convexity, the well-developed paradigms convex optimization cannot be fully extended here, leading to the current situation that the theory of non-convex optimization is way behind the practice. In this mini-symposium, we focus on recent advances in non-convex optimization, including the analysis and understanding of the fundamental nature of the non-convex optimization, algorithmic bias/implicit regularization of gradient-based algorithms, fast convergent algorithms in non-convex problems, and their applications in inverse problems, imaging and machine learning and many others.

**Organizer(s) :** Guoyin Li, Jingwei Liang, Junqi Tang

part\_1

**Classification :** 90C26, 65K05, 49M37, 90C35, 90C30**Minisymposium Program :**

00521 (1/5) : 3D @A206 [Chair: Guoyin Li]

**[02446] Convergence rate analysis of a Dykstra-type projection algorithm****Format :** Talk at Waseda University**Author(s) :** Xiaozhou Wang (The Hong Kong Polytechnic University)Ting Kei Pong (The Hong Kong Polytechnic University)**Abstract :** We extend the Dykstra's projection algorithm to find projections onto the intersection of linear preimages of closed convex sets. The algorithm only makes use of projections onto the latter sets and operations by the linear maps and their adjoints in every iteration. Explicit convergence rate is derived when each set is  $C^{1,\alpha}$ -cone reducible for some  $\alpha \in (0, 1]$ , under standard relative interior conditions. Concrete examples are constructed to illustrate the necessity of some of our assumptions.**[04336] Critical points of the projection onto the set of low rank tensors****Format :** Talk at Waseda University**Author(s) :** Shenglong Hu (Hangzhou Dianzi University)**Abstract :** In 2009, SIAM von Neumann prize-winner Yousef Saad proposed the open problem on characterizing the convergence rate of the classical alternating polar decomposition method for low rank orthogonal tensor approximation problem. Actually, this problem was initiated by Gene Golub in 2001 for the rank one case, and received considerable study in the past twenty years. In 2015, concrete examples were given showing that the convergence rate may be sublinear, linear and superlinear. In this talk, we show that for a generic tensor, the algorithm converges linearly without any further assumption by studying the critical points of the projection onto the set of low rank tensors.**[05256] Nonconvex Semi-algebraic Optimization: From Exact to Convergent Conic Program Relaxations****Format :** Talk at Waseda University**Author(s) :** Jeya Jeyakumar (UNSW Sydney)**Abstract :** Semi-algebraic optimization is the study of optimization problems where the feasible set is defined in terms of polynomial inequalities, called a semi-algebraic set. In addition to the usual tools of nonlinear optimization, such as convex analysis and linear algebra, powerful techniques of real algebraic geometry, such as representation theorems for polynomials, and conic programming methods, such as semi-definite programming and copositive programming, can be employed to study these problems. In this talk, I will describe the key results in this area, highlighting our recent work on the development of exact conic programming relaxations and convergent hierarchy of conic programming relaxations for classes of semi-algebraic optimization problems.

00521 (2/5) : 3E @A206 [Chair: Guoyin Li]

**[01258] Global convergence of the gradient method for functions definable in o-minimal structures****Format :** Talk at Waseda University**Author(s) :** Cedric Josz (Columbia University)**Abstract :** We consider the gradient method with variable step size for minimizing functions that are definable in o-minimal structures on the real field and differentiable with locally Lipschitz gradients. A sufficient condition ensuring global convergence is discussed, with implications for the convergence rate and convergence to a local minimum. Applications include principal component analysis, matrix sensing, and linear neural networks.**[04681] Convergence theory for mean-field optimization methods****Format :** Talk at Waseda University**Author(s) :** Atsushi Nitanda (Kyushu Institute of Technology)Denny Wu (University of Toronto)Taiji Suzuki (The University of Tokyo)**Abstract :** Optimization of mean-field models recently attracts attention due to its connection to training two-layer neural networks under the mean-field regime. To analyze the optimization dynamics of mean-field models, we have established the theory of convex analysis and have derived several optimization methods. In this talk, we present recent advances in the theory for mean-field optimization methods.

## [03322] Convergence Theorem for Deep Neural Network with ReLU Activation

**Format :** Talk at Waseda University

**Author(s) :** Gue Myung Lee (Department of Applied Mathematics, Pukyong National University)Jae Hyoung Lee (Department of Applied Mathematics, Pukyong National University)Kwang Baik Lee (Department of Applied Mathematics, Pukyong National University)

**Abstract :** Deep Neural Network (Deep Learning) is an artificial neural network which consists of input layer, output layer and many hidden layers between them. The gradient descent algorithm is the key one in the learning system for the deep neural network. So, for understanding the learning system, we should know the convergence for the descent algorithm for the cost function of L-layers neural network. The cost function is a composition of weight variables, biases variables and activation functions.

In this talk, we consider the convergence theorem for the descent algorithm for the cost function of L-layers neural network with ReLU function( $\sigma(z) = \max\{0, z\}$ ) as its activation function. First, we show that the cost function is semi-algebraic and locally Lipschitz. Secondly, we show that the sequence, which was generated by the descent algorithm with Clarke generalized gradient, globally converges to a stationary point (critical point) under certain assumptions. Thirdly, we prove that the set of critical values of the cost function is finite.

## [05068] Theoretical and practical applications of signomial rings to polynomial optimization

**Format :** Talk at Waseda University

**Author(s) :** Mareike Dressler (UNSW Sydney)

**Abstract :** Signomials generalize polynomials by allowing arbitrary real exponents, at the expense of restricting the resulting function to the positive orthant. In this talk, I present a signomial Positivstellensatz based on conditional "sums of arithmetic-geometric exponentials" (SAGE). The Positivstellensatz applies to compact sets which need not be convex or even basic semi-algebraic. In the first part of the talk, I explain how this result is derived through the newly-defined concept of signomial rings. Then I show how the same concept leads to a novel convex relaxation hierarchy of lower bounds for signomial optimization. These relaxations (which are based on relative entropy programming) can be solved more reliably than those arising from earlier SAGE-based Positivstellensätze. Moreover, this increase in reliability comes at no apparent cost of longer solver runtimes or worse bounds. Numerical examples are provided to illustrate the performance of the hierarchy on a problem in chemical reaction networks.

This talk is based on joint work with Riley Murray.

00521 (3/5) : 4C @A206 [Chair: Jingwei Liang]

## [04380] Proximal methods for nonsmooth and nonconvex fractional programs: when sparse optimization meets fractional programs

**Format :** Talk at Waseda University

**Author(s) :** Guoyin Li (University of new south wales )Radu Ioan Bot (University of Vienna)Minh Dao (Royal Melbourne Institute of Technology)

**Abstract :** Nonsmooth and nonconvex fractional programs are ubiquitous and also highly challenging. It includes the composite optimization problems studied extensively lately, and encompasses many important modern optimization problems arising from diverse areas such as the recent proposed scale invariant sparse signal reconstruction problem in signal processing, the robust Sharpe ratio optimization problems in finance and the sparse generalized eigenvalue problem in discrimination analysis. In this talk, we will introduce extrapolated proximal methods for solving nonsmooth and nonconvex fractional programs and analyse their convergence behaviour. Interestingly, we will show that the proposed algorithm exhibits linear convergence for sparse generalized eigenvalue problem with either cardinality regularization or sparsity constraints. This is achieved by identifying the explicit desingularization function of the Kurdyka-Łojasiewicz inequality for the merit function of the fractional optimization models. Finally, if time permits, we will present some preliminary encouraging numerical results for the proposed methods for sparse signal reconstruction and sparse Fisher discriminant analysis.

## [03321] Error bounds based on facial residual functions

**Format :** Talk at Waseda University

**Author(s) :** Bruno Lourenço (Institute of Statistical Mathematics)Scott B. Lindstrom (Curtin University)Ting Kei Pong (The Hong Kong Polytechnic University)

**Abstract :** In this talk, we overview some recent error bound results obtained under the framework of facial residual functions.

This includes new tight error bounds for optimization problems with constraints involving exponential cones, p-cones and others. Time allowing, we will briefly illustrate the applications of such results in proving precise convergence rates of certain algorithms and in determining automorphism groups of cones.

## [02798] Doubly majorized algorithm for sparsity-inducing optimization problems with regularizer-compatible constraints

**Format :** Talk at Waseda University

**Author(s) :** Tianxiang Liu (Tokyo Institute of Technology )Ting Kei Pong (The Hong Kong Polytechnic University)Akiko Takeda (The University of Tokyo)

**Abstract :** We consider a class of sparsity-inducing optimization problems whose constraint set is regularizer-compatible. By exploiting absolute-value symmetry and other properties in the regularizer, we propose a new algorithm, called the Doubly Majorized Algorithm (DMA). Without invoking any commonly used constraint qualification conditions, we show that the sequence generated by DMA clusters in a new stationary point inspired by the notion of L-stationarity. Finally, numerical performance of DMA on variants of ordered LASSO is also illustrated.

00521 (4/5) : 4D @A206 [Chair: Jingwei Liang]

## [04271] Differentiating Nonsmooth Solutions to Parametric Monotone Inclusion Problems

**Format :** Talk at Waseda University

**Author(s) :** Antonio José Silveti-Falls (Université Paris-Saclay, CentraleSupélec, INRIA OPIS, France)Edouard Pauwels (Université Toulouse 3 Paul Sabatier)Jérôme Bolte (Université Toulouse Capitole, Toulouse School of Economics)

**Abstract :** Understanding the differentiability and regularity of the solution to a monotone inclusion problem is an important question with consequences for convex optimization, machine learning, signal processing, and beyond. Past attempts have been made either under very restrictive assumptions that ensure the solution is continuously differentiable or using mathematical tools that are incompatible with automatic differentiation. In this talk, we discuss how to leverage path differentiability and a recent result on nonsmooth implicit differentiation calculus to give sufficient conditions ensuring that the solution to a monotone inclusion problem will be path differentiable and provide formulas for computing its generalized gradient. Our approach is fully compatible with automatic differentiation and comes with assumptions which are easy to check, roughly speaking: semialgebraicity and strong monotonicity. We illustrate the scope of our results by considering three fundamental composite problem settings: strongly convex problems, dual solutions to convex minimization problems and primal-dual solutions to min-max problems.

## [01315] Optimal Neural Network Approximation of Wasserstein Gradient Direction via Convex Optimization

**Format :** Online Talk on Zoom

**Author(s) :** Yifei Zack Wang (Stanford University)Peng Chen (Georgia Institute of Technology)Mert Pilanci (Stanford University)Wuchen Li (University of South Carolina)

**Abstract :** The computation of Wasserstein gradient direction is essential for posterior sampling problems and scientific computing. For finite samples, we approximate the score function in the family of two-layer networks with squared-ReLU activations. We derive a semi-definite programming (SDP) relaxation of the variational problem, which can be efficiently solved by standard interior point method. Numerical experiments including PDE-constrained Bayesian inference and parameter estimation in COVID-19 modeling demonstrate the effectiveness of the proposed method.

## [01537] Data-informed deep optimization

**Format :** Talk at Waseda University

**Author(s) :** Lulu Zhang (Shanghai Jiao Tong University)

**Abstract :** Motivated by the impressive success of deep learning, we explore the application of deep learning into a specific class of optimization problems lacking explicit formulas for both objective function and constraints. In this work, we propose a data-informed deep optimization (DiDo) approach emphasizing on the adaptive fitting of the feasible region. To demonstrate the effectiveness of our DiDo approach, we consider a practical design case in industry and a 100-dimension toy example.

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00521 (5/5) : 4E @A206 [Chair: Jingwei Liang]

## [02734] Continuous Newton-like Methods featuring Inertia and Variable Mass

**Format :** Talk at Waseda University

**Author(s) :** Camille Castera (University of Tübingen)Hedy Attouch (IMAG, Université Montpellier, CNRS)Jalal Fadili (ENSICAEN, Normandie Université, CNRS, GREYC)Peter Ochs (University of Tübingen)

**Abstract :** Towards designing new algorithms that benefit from the best of both first- and second-order optimization methods, we introduce a new dynamical system, called VM-DIN-AVD, at the interface between second-order dynamics with inertia and Newton's method. This system extends the class of inertial Newton-like dynamics by featuring a time-dependent parameter in front of the acceleration, called variable mass. For strongly convex optimization, we provide guarantees on how the Newtonian and inertial behaviors of the system can be non-asymptotically controlled by means of this variable mass. A connection with the Levenberg-Marquardt --or regularized Newton's-- method is also made. We then show the effect of the variable mass on the asymptotic rate of convergence of the dynamics, and in particular, how it can turn the latter into an accelerated Newton method. We present numerical experiments supporting our findings.

## [01611] Inertial quasi-Newton methods for monotone inclusion

**Format :** Talk at Waseda University

**Author(s) :** Shida Wang (Universität Tübingen)Jalal Fadili (Normandie Univ, ENSICAEN)Peter Ochs (Universität Tübingen)

**Abstract :** We introduce an inertial quasi-Newton Forward-Backward Splitting Algorithm to solve a class of monotone inclusion problems. While the inertial step is computationally cheap, in general, the bottleneck is the evaluation of the resolvent operator. A change of the metric makes its computation hard even for (otherwise in the standard metric) simple operators. In order to fully exploit the advantage of adapting the metric, we develop a new efficient resolvent calculus for a low-rank perturbed standard metric, which accounts exactly for quasi-Newton metrics. Moreover, we prove the convergence of our algorithms, including linear convergence rates in case one of the two considered operators is strongly monotone. Beyond the general monotone inclusion setup, we instantiate a novel inertial quasi-Newton Primal-Dual Hybrid Gradient Method for solving saddle point problems. The favourable performance of our inertial quasi-Newton PDHG method is demonstrated on several numerical experiments in image processing.

## [05250] Extrapolated Proximal Algorithms for Nonconvex and Nonsmooth Min-max problems

**Format :** Talk at Waseda University

**Author(s) :** Peter Wu (UNSW)Guoyin Li (The University of New South Wales)Minh Dao (RMIT)

**Abstract :** In this talk, we consider an extrapolated proximal algorithm for solving nonsmooth and nonconvex minmax problems. We establish convergence of the full sequence to a stationary point under some gentle assumptions. If time permits, numerical experiment on its application to multi-domain robust sparse learning will be presented.

## [05578] Global stability of first-order methods for coercive tame functions

**Format :** Talk at Waseda University

**Author(s) :** Cédric Josz (Columbia University)Lexiao Lai (Columbia University)

**Abstract :** We consider first-order methods with constant step size for minimizing locally Lipschitz coercive functions that are tame in an o-minimal structure on the real field. We prove that if the method is approximated by subgradient trajectories, then the iterates eventually remain in a neighborhood of a connected component of the set of critical points. Under suitable model-dependent regularity assumptions, this result applies to the random reshuffling and momentum and the random-permutations cyclic coordinate descent method.

## [00523] Implicit methods for hyperbolic problems and their extensions and applications

**Session Time & Room :**

00523 (1/3) : 3C (Aug.23, 13:20-15:00) @A618

00523 (2/3) : 3D (Aug.23, 15:30-17:10) @A618

00523 (3/3) : 3E (Aug,23, 17:40-19:20) @A618

**Type :** Proposal of Minisymposium

**Abstract :** Hyperbolic partial differential equations and their numerical solutions play an important role in several fields of applied mathematics. Many interesting applications of related PDEs are stiff in nature, so implicit time discretizations with enhanced stability properties are good candidates for their numerical solution. The minisymposium shall discuss important aspects of such methods like higher order accuracy, non-oscillatory behavior, well-balancing, asymptotic-preserving, efficient solvers, and combinations with explicit schemes.

**Organizer(s) :** Peter Frolkovič, Pep Mulet, Carlos Parés

**Classification :** 35L04

**Minisymposium Program :**

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00523 (1/3) : 3C @A618 [Chair: Carlos Parés]

## [04131] Semi-implicit schemes for a convection-diffusion-reaction model of sequencing batch reactors

**Format :** Talk at Waseda University

**Author(s) :** Raimund Bürger (Universidad de Concepción)Julio Careaga (Radboud University)Stefan Diehl (Lund University)Romel Pineda (Universidad de Concepción)

**Abstract :** Sequencing batch reactors are used in wastewater treatment for the settling of solid biomass particles simultaneously with biochemical reactions with nutrients dissolved in the liquid. This unit can be modeled as a moving-boundary problem for a degenerating convection-diffusion-reaction system. This model is transformed to a fixed computational domain and is discretized by an explicit and semi-implicit monotone schemes. Both variants obey an invariant region property. Numerical examples illustrate that the semi-implicit variant is more efficient.

## [01691] High resolution well-balanced compact implicit numerical scheme for numerical solution of the shallow water equations

**Format :** Talk at Waseda University

**Author(s) :** Michal Žeravý (Slovak University of Technology in Bratislava)Peter Frolkovič (Slovak University of Technology in Bratislava)

**Abstract :** In this talk, we deal with the numerical solution of shallow water equations with topography in one-dimensional case using a high resolution well-balanced compact implicit numerical scheme. The upwind scheme uses the fractional step method with the fast sweeping method. Consequently, the Jacobian matrix of the discrete system of nonlinear algebraic equations is always either a lower or upper triangular matrix.

## [01692] Numerical solution of scalar hyperbolic problems using the third order accurate compact implicit scheme

**Format :** Talk at Waseda University

**Author(s) :** Dagmar Zakova (Slovak University of Technology in Bratislava)Peter Frolkovic (Slovak University of Technology in Bratislava)

**Abstract :** This work presents compact implicit numerical schemes for solving scalar hyperbolic problems. We propose details of the third-order accurate scheme using the finite volume method. To avoid unphysical oscillations in the case of nonsmooth solution, we modify the scheme using ENO and WENO approximation in space. Applications to one-dimensional conservation laws are shown.

## [05425] High-fidelity multiderivative time integration for compressible flows

**Format :** Talk at Waseda University

**Author(s) :** Arjun Thenery Manikantan (Hasselt University)Jochen Schütz (Hasselt University)Jonas Zeifang (Hasselt University)

**Abstract :** We present a high-order parallel-in-time implicit multiderivative time-stepping scheme for Navier Stokes equations spatially discretized with the Discontinuous Galerkin Spectral element method. The time-stepping starts with a predicted solution, and the correction steps increase the order of accuracy up to the order of the underlying quadrature rule. Implicit non-linear(linear) equations are solved using Newton's and the general minimal residual methods. Extensive numerical results are shown for convergence, parallel efficiency, and other scheme features.

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00523 (2/3) : 3D @A618 [Chair: Pep Mulet]

## [01684] Implicit and semi-implicit well-balanced finite volume methods for general 1d systems of balance laws

**Format :** Talk at Waseda University

**Author(s) :** Carlos Parés (University of Málaga)Irene Gómez-Bueno (University of Málaga)Manuel Jesús Castro (University of Málaga)Sebastiano Boscarino (University of Catania)Giovanni Russo (University of Catania)

**Abstract :** In this work a general family of implicit and semi-implicit well-balanced finite volume numerical methods for nonlinear hyperbolic systems of balance laws will be presented. These methods are obtained by extending a general strategy introduced by some of the authors to design high-order well-balanced explicit methods. This strategy, based on the computation of local steady states, will be combined with implicit RK or IMEX solvers in time. Different applications will be shown.

## [01665] SHALLOW-WATER MODEL: IMPLICIT FULLY WELL-BALANCED METHODS IN THE LAGRANGE-PROJECTION FRAMEWORK

**Format :** Talk at Waseda University

**Author(s) :** Celia Caballero Cárdenas (Universidad de Málaga)Manuel Jesús Castro Díaz (Universidad de Málaga)Tomás Morales de Luna (Universidad de Malaga)María de la Luz Muñoz-Ruiz (Universidad de Málaga)Christophe Chalons (Université Versailles Saint-Quentin-en-Yvelines)

**Abstract :** We propose fully well-balanced Lagrange-Projection finite volume schemes for the shallow-water model. This two-step approach separates acoustic and transport phenomena, allowing for implicit-explicit and large time step schemes with CFL restriction based on slower transport waves.

## [01664] Hyperbolic systems with stiff relaxation: asymptotic-preserving and well-balanced schemes

**Format :** Talk at Waseda University

**Author(s) :** Irene Gómez-Bueno (University of Málaga)Sebastiano Boscarino (University of Catania)Manuel Jesús Castro Díaz (University of Málaga)Carlos Parés (University of Málaga)Giovanni Russo (University of Catania)

**Abstract :** We consider hyperbolic systems depending on a stiff parameter  $\varepsilon$ : when  $\varepsilon$  is small, numerical schemes may produce spurious results. Implicit-explicit Runge-Kutta schemes have been widely used for their time evolution. Our goal is to design high-order asymptotic-preserving methods which are at the same time well-balanced for the asymptotic limit system.

## [01673] MIRK methods and applications in RRMHD and neutrino transport equations

**Format :** Talk at Waseda University

**Author(s) :** Isabel Cordero-Carrión (University of Valencia)Samuel Santos-Pérez (University of Valencia)Martin Obergaulinger (University of Valencia)

**Abstract :** We present the Minimally-Implicit Runge-Kutta (MIRK) methods for the numerical resolution of hyperbolic equations with stiff source terms. We apply these schemes to the resistive relativistic magnetohydrodynamic (RRMHD) and the M1 neutrino transport equations. Previous approaches rely on Implicit-Explicit Runge-Kutta schemes. The MIRK methods are able to deal with stiff terms producing stable numerical evolutions and their computational cost is similar to the standard explicit methods.

00523 (3/3) : 3E @A618 [Chair: Peter Frolkovič]

## [03904] Implicit-explicit schemes for Cahn-Hilliard-Navier-Stokes equations

**Format :** Talk at Waseda University

**Author(s) :** Pep Mulet (University of Valencia)

**Abstract :** Navier-Stokes-Cahn-Hilliard equations are a system of fourth-order partial differential equations that model the evolution of compressible mixtures of binary fluids (e.g. foams, solidification processes, fluid-gas interface) under gravitational effects. Our aim is to use implicit-explicit time-stepping schemes to avoid the severe restriction posed by the high order terms for the efficient numerical solution of problems with these equations.

# [00524] Lie Symmetries, Solutions and Conservation laws of nonlinear differential equations

## **Session Time & Room :**

00524 (1/4) : 1C (Aug.21, 13:20-15:00) @A201

00524 (2/4) : 1D (Aug.21, 15:30-17:10) @A201

00524 (3/4) : 1E (Aug.21, 17:40-19:20) @A201

00524 (4/4) : 2C (Aug.22, 13:20-15:00) @A201

## **Type :** Proposal of Minisymposium

**Abstract :** This mini-symposium is devoted to all research areas that are related to nonlinear differential equations and their applications in science and engineering. The main focus of this mini-symposium is on the Lie symmetry analysis, conservation laws and their applications to ordinary and partial differential equations. These differential equations could originate from mathematical models of diverse disciplines such as architecture, chemical kinetics, civil engineering, ecology, economics, engineering, fluid mechanics, biology and finance. Other approaches in finding exact solutions to nonlinear differential equations will also be discussed. This includes, but not limited to, asymptotic analysis methodologies, bifurcation theory, inverse scattering transform techniques, the Hirota method, the Adomian decomposition method, and others.

**Organizer(s) :** Chaudry Masood Khalique

**Classification :** 35B06, 35L65, 35C05, 35C08, 70S05

## **Minisymposium Program :**

00524 (1/4) : 1C @A201 [Chair: Carel Olivier]

# [02723] Conservation laws and variational structure of damped nonlinear wave equations

## **Format :** Talk at Waseda University

**Author(s) :** Almudena P. Márquez (University of Cadiz)Stephen Anco (Brock University)Tamara M. Garrido (University of Cadiz)María L. Gandarias (University of Cadiz)

**Abstract :** All low-order conservation laws are found for a general class of nonlinear wave equations in one dimension with linear damping which is allowed to be time-dependent. Such equations arise in numerous physical applications and have attracted much attention in analysis. The conservation laws describe generalized momentum and boost momentum, conformal momentum, generalized energy, dilational energy, and light-cone energies. Both the conformal momentum and dilational energy have no counterparts for nonlinear undamped wave equations in one dimension. All of the conservation laws are obtainable through Noether's theorem, which is applicable because the damping term can be transformed into a time-dependent self-interaction term by a change of dependent variable. For several of the conservation laws, the corresponding variational symmetries have a novel form which is different than any of the well known variation symmetries admitted by nonlinear undamped wave equations in one dimension.

# [03330] Constructing mass-conserving cnoidal wave solutions for the KdV equation

## **Format :** Talk at Waseda University

**Author(s) :** Carel Petrus Olivier (North-West University)Frank Verheest (Universiteit Gent)

**Abstract :** Nonlinear periodic travelling wave solutions of the Korteweg-deVries (KdV) equation in the form of cnoidal wave solutions are investigated. The general cnoidal wave solution does not ensure that the mass of the undisturbed medium is conserved. In this paper, a framework is provided to construct mass-conserving cnoidal wave solutions., and the resulting solutions are analyzed. It is shown that these solutions are consistent with linear solutions in the small amplitude limit.

## [04290] Conservation laws and symmetries of a Generalized Drinfeld-Sokolov system

**Format :** Talk at Waseda University

**Author(s) :** Tamara M. Garrido (University of Cadiz)Rafael De La Rosa (University of Cadiz)Elena Recio (University of Cadiz)Almudena P. Márquez (University of Cadiz)

**Abstract :** The generalized Drinfeld-Sokolov system is a widely-used model that describes wave phenomena in various contexts. Many properties of this system, such as Hamiltonian formulations and integrability, have been extensively studied, and exact solutions have been derived for specific cases. In this paper, we apply the direct method of multipliers to obtain all low-order local conservation laws of the system. These laws correspond to physical quantities that remain constant over time, such as energy and momentum, and we provide a physical interpretation for each of them. Additionally, we investigate the Lie point symmetries and first-order symmetries of the system. Through the point symmetries and constructing the optimal systems of one-dimensional subalgebras, we are able to reduce the system of partial differential equations to ordinary differential systems.

## [02959] Lie symmetry analysis of flow and pressure inside horizontal chamber

**Format :** Talk at Waseda University

**Author(s) :** Tanki Motsepa (University of Mpumalanga)Modisawatsona Lucas Lekoko (North-West University)Gabriel Magalakwe (North-West University)

**Abstract :** Exact solutions improve industrial processes by giving operators greater grasp of how systems operate. The study aims to find exact momentum and pressure solutions during the unsteady filtration process. Lie symmetry analysis is used to transform a system of PDEs representing the case study into solvable ODEs. The ODEs are then solved to obtain velocity and pressure solutions. Effects of parameters resulting from the dynamics are examined to identify the parameters that yield maximum outflow.

00524 (2/4) : 1D @A201 [Chair: Tanki Motsepa]

## [03457] Closed-form solutions and conservation laws of the fifth-order strain wave equation in microstructured solids

**Format :** Online Talk on Zoom

**Author(s) :** Mduduza Thabo Lephoko (North-West University, Mafikeng Campus)Chaudry Masood Khalique (North-West University, South Africa)

**Abstract :** In this presentation, we examine the dynamics of soliton waves associated with higher-order nonlinear partial differential equations, which have applications in various fields of science and engineering. Our focus is on the fifth-order strain wave equation, for which we employ the Lie group theory of differential equations to obtain analytic solutions. Specifically, we use this technique to systematically generate the Lie point symmetries spanned by the equation, which we then use to reduce it to ordinary differential equations that can be solved to obtain closed-form solutions. The ordinary differential equations are solved by direct integration and the engagement of two methods, the simplest method and generalized tanh-function method. We successfully identify soliton solutions, including dark and singular period solitons, and depict them graphically to better understand their physical meaning. We then use the multiplier method to obtain conserved vectors. Our analysis sheds light on the wave structures associated with the strain wave equation and provides insight into the physical implications of the soliton solutions.

## [02308] Symmetry solutions and conservation laws of the derivative nonlinear Schrodinger equation

**Format :** Online Talk on Zoom

**Author(s) :** Karabo Plaatjie (North-West University, Mafikeng Campus)Chaudry Masood Khalique (North-West University, South Africa)

**Abstract :** In this talk we study the derivative nonlinear Schrodinger equation. This equation has many applications, for example in the propagation of circular polarized nonlinear Alfvén waves in plasmas. We present general and special solutions of this equation using Lie group theory. We also derive conservation laws for the underlying equation.

## [03449] Lie symmetry analysis of new 3-D fifth-order nonlinear Wazwaz equation

**Format :** Online Talk on Zoom

**Author(s) :** Oke Davies Adeyemo (North-West University, Mafikeng Campus)

**Abstract :** In this talk, we present the analytical examination of a new (3+1)-dimensional fifth-order nonlinear Wazwaz equation with third-order dispersion terms in ocean physics and other nonlinear sciences. We apply Lie group analysis to obtain various infinitesimal generators admitted by the equation. The generators are used to reduce the understudy

part\_1

equation to achieve copious group-invariant solutions. Thus, various closed-form solutions are obtained for the equation. We further construct its conservation laws.

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00524 (3/4) : 1E @A201 [Chair: C M KHALIQUE]

### **[03451] Lie group analysis of the nonlinear 3D KP-BBM equation**

**Format :** Online Talk on Zoom

**Author(s) :** Jonathan Lebogang Bodibe (North-West University, Mafikeng Campus)Chaudry Masood Khalique (North-West University, South Africa)

**Abstract :** In this talk, we present Lie group analysis of the nonlinear (3+1)-dimensional Kadomtsev Petviashvili Benjamin Bona Mahony equation. We find exact solutions of the equation using Lie symmetry method together with Kudryashov's and  $(G'/G)$ -expansion methods. Moreover, we derive the conservation laws for the equation using the multiplier and Ibragimov's methods.

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00524 (4/4) : 2C @A201 [Chair: C M KHALIQUE]

### **[04488] Integrable equations and Riemann-Hilbert problems**

**Format :** Talk at Waseda University

**Author(s) :** Wen-Xiu Ma (University of South Florida)

**Abstract :** This talk covers the zero curvature formulation and the Riemann-Hilbert technique. Nonlocal integrable equations are derived from conducting group reductions. The associated matrix spectral problems are used to build a kind of Riemann-Hilbert problems, whose reflectionless cases generate soliton solutions.

### **[04064] A study of 3D generalized nonlinear wave equation in fluids**

**Format :** Talk at Waseda University

**Author(s) :** Chaudry Masood Khalique (North-West University, South Africa)

**Abstract :** In this talk we study a (3+1)-dimensional generalized nonlinear wave equation of fluids. Using Lie symmetry methods, we transform the underlying equation into a nonlinear ordinary differential equation. We deduce periodic, trigonometric bright soliton together with singular soliton solutions. Moreover, some soliton solutions are secured via the simplest equation method in the form of Jacobi elliptic functions. The dynamics of the solutions are depicted using suitable graphs. Furthermore, we construct conservation laws of the equation by employing Ibragimov's theorem.

### **[04126] Burgers' nth Partial Differential Equation Hierarchy**

**Format :** Talk at Waseda University

**Author(s) :** Sameerah Jamal (University of the Witwatersrand )

**Abstract :** We present some recent advances of the applications of one-parameter Lie group transformations of famous partial differential equations. In particular, we discuss the Burgers' equation, which are often the benchmarks in the study of differential equations. We exploit the link between the equation and a recursion operator and show how the full hierarchy may be solved.

### **[03471] Nonclassical Potential Symmetries for the transient heat transfer equation**

**Format :** Talk at Waseda University

**Author(s) :** Mpho Nkwanazana (Sefako Makgatho Health Science University)Raseelo Moitsheki (University of the Witwatersrand)

**Abstract :** In this article we consider the one dimensional transient heat conduction equation. The diffusivity term and internal heat generator are given by the power law. The objective is to employ nonclassical and nonlocal approach to generate nonclassical potential symmetries.

# [00528] High order and well-balanced methods and stability analysis for non-linear hyperbolic systems

**Session Time & Room :**

00528 (1/2) : 1C (Aug.21, 13:20-15:00) @G606

00528 (2/2) : 1D (Aug.21, 15:30-17:10) @G606

**Type :** Proposal of Minisymposium

**Abstract :** Many complex physical phenomena may be modeled by means of non-linear hyperbolic systems. When approximating such systems, one requires the use of efficient, accurate and stable numerical schemes. On the one hand, the use of high-order methods will be necessary in order to reduce the numerical diffusion inherent to the numerical approach. On the other hand, it is common for these systems the existence of some particular steady-state solutions that should be preserved, which will need the use of a well-balanced scheme.

The goal of this mini-symposium is the discussion and presentation of state-of-the-art computational and numerical methods of high-order well-balanced schemes with applications to hyperbolic systems.

**Organizer(s) :** Tomas Morales de Luna, Ernesto Guerrero-Fernandez

**Classification :** 35L60, 76M12, 35L45, 76B15

**Minisymposium Program :**

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00528 (1/2) : 1C @G606 [Chair: Tomas Morales de Luna]

## [01682] High order well-balanced finite volume and discontinuous Galerkin schemes for a first order hyperbolic reformulation of the coupled Einstein-Euler system in 3+1 general relativity

**Format :** Talk at Waseda University

**Author(s) :** Michael Dumbser (University of Trento)

**Abstract :** We present new well-balanced finite volume and discontinuous Galerkin schemes for the solution of a new first order hyperbolic Z4 formulation of the Einstein-Euler system of general relativity. Nonlinear involutions are accounted for via a covariant GLM cleaning technique. We introduce a new, simple and efficient type of well-balancing that automatically applies to any numerical discretization and arbitrary equilibria in multiple space dimensions. We show numerical results for vacuum spacetimes and for a TOV star.

## [01699] Numerical approximation of non-convex relativistic hydrodynamics

**Format :** Talk at Waseda University

**Author(s) :** Susana Serna (Universitat Autonoma de Barcelona)Antonio Marquina (Universidad de Valencia)

**Abstract :** We explore the rich and complex dynamics that a phenomenological equation of state (EoS) with non-convex regions in the pressure-density plane may develop as a result of genuinely relativistic effects. We study the parameter space of the EoS to ensure its causality and thermodynamical consistency. We approximate the non-conventional dynamics developed in the evolution of relativistic blast waves by means of a high order shock capturing scheme.

## [01720] Recovering primitive variables in special relativistic hydrodynamics

**Format :** Talk at Waseda University

**Author(s) :** Antonio Marquina (Universidad de Valencia)Susana Serna (Universitat Autonoma de Barcelona)Jose M Ibanez (Universidad de Valencia)

**Abstract :** We study an iterative procedure based on fixed-point strategy to recover primitive variables in each time step of the evolution of Special Relativistic Hydrodynamic equations. Given a set of three conserved values we start the iteration by prescribing an initial zero pressure so that if the first iterate is strictly positive, then, the fixed-point iteration monotonically converges to the unique pressure associated to the conserved variables.

## [01290] Well-Balanced High-Order Discontinuous Galerkin Methods for Systems of Balance Laws

**Format :** Talk at Waseda University

**Author(s) :** Ernesto Guerrero Fernández (National Oceanic and Atmospheric Administration (NOAA))Cipriano Escalante Sanchez (Universidad de Málaga)Manuel Castro Díaz (Universidad de Málaga)

**Abstract :** This work introduces a general strategy to develop well-balanced high-order Discontinuous Galerkin (DG) numerical schemes for systems of balance laws. The essence of our approach is a local projection step that guarantees the exactly well-balanced character of the resulting numerical method for smooth stationary solutions. The strategy can be adapted to some well-known different time marching DG discretisations. Particularly, in this article, Runge-Kutta DG and ADER DG methods are studied. Additionally, a limiting procedure based on a modified WENO approach is described to deal with the spurious oscillations generated in the presence of non-smooth solutions, keeping the well-balanced properties of the scheme intact. The resulting numerical method is then exactly well-balanced and high-order in space and time for smooth solutions. Finally, some numerical results are depicted using different systems of balance laws to show the performance of the introduced numerical strategy.

00528 (2/2) : 1D @G606 [Chair: Ernesto Guerrero Fernández]

## [01687] Structure preserving high order discontinuous Galerkin schemes for general relativity

**Format :** Talk at Waseda University

**Author(s) :** Elena Gaburro (Inria)Michael Dumbser (University of Trento)Ilya Peshkov (University of Trento)Olindo Zanotti (University of Trento)Manuel J. Castro (University of Malaga)

**Abstract :** In this talk we present a novel first order hyperbolic reformulation of the coupled Einstein-Euler system allowing robust and long-time stable simulations for the joint evolution of matter and space-time in general relativity. Among our numerical results we have long-time evolution of TOV neutron stars and accretion disks and a black holes collision. This is obtained through high order discontinuous Galerkin schemes endowed with subcell finite volume limiter, well balanced techniques and GLM curl cleaning.

## [01663] Multidimensional approximate Riemann solvers for hyperbolic nonconservative systems

**Format :** Talk at Waseda University

**Author(s) :** José M. Gallardo (University of Málaga)

**Abstract :** This work deals with the development of efficient incomplete multidimensional Riemann solvers for hyperbolic systems. We present a general strategy for constructing genuinely two-dimensional Riemann solvers, that can be applied for solving systems including source and coupling terms. Two-dimensional effects are taken into account through the approximate solutions of 2d Riemann problems arising at the vertices of the computational mesh. Applications to magnetohydrodynamics and shallow water equations are presented.

## [01841] A fully-well-balanced hydrodynamic reconstruction

**Format :** Talk at Waseda University

**Author(s) :** Christophe Berthon (Nantes Université)Victor Michel-Dansac (INRIA)

**Abstract :** The present work concerns the numerical approximation of the weak solutions of the shallow-water model. To address such an issue, the well-known hydrostatic reconstruction is adopted. Such a relevant technique easily gives numerical schemes able to exactly capture the steady states at rest. Here, necessary conditions are stated on the reconstruction process in order to also capture the moving steady states. An example of suitable hydrodynamic reconstruction is presented and tested.

## [01690] A well-balanced scheme for landslide models

**Format :** Talk at Waseda University

**Author(s) :** Manuel J. Castro (Universidad de Málaga)Cipriano Escalante Sanchez (Universidad de Málaga)José Garres-Díaz (Universidad de Córdoba, Spain)Tomas Morales de Luna (Universidad de Málaga)

**Abstract :** When landslide models in the shallow water framework, special care has to be taken with the stationary solutions. Indeed, motion of the material only begins when the slope of the material is bigger than that of the repose angle. Preserving such steady states is not a trivial task. We present here different strategies to design well-balance high-order finite volume schemes.

# [00529] Numerical approximation of geophysical flows

**Session Time & Room :**

00529 (1/2) : 1E (Aug.21, 17:40-19:20) @G606

00529 (2/2) : 2C (Aug.22, 13:20-15:00) @G606

**Type :** Proposal of Minisymposium

**Abstract :** Hyperbolic PDE systems naturally appear in many real-world applications, particularly in geophysical flow models. They are of essential importance for understanding natural phenomena and for their prediction.

This mini-symposium focuses on geophysical flows with a particular interest in the shallow water framework and related applications such as sediment transport, tsunami hazards, and viscoplastic flows.

The objective will be to discuss and presents new trends in computational and numerical methods for shallow flows and their applications.

**Organizer(s) :** Cipriano Escalante, José Garres

**Classification :** 35L60, 76M12, 35L45, 76U60

**Minisymposium Program :**

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00529 (1/2) : 1E @G606 [Chair: José Garres]

## [01506] Monotonicity-preserving interpolation in multilevel schemes for balance laws

**Format :** Talk at Waseda University

**Author(s) :** Antonio Baeza (University of Valencia, Spain)Rosa Donat (University of Valencia)Anna Martínez-Gavara (University of Valencia)

**Abstract :** This work deals with the problem of developing cost-effective multilevel schemes for balance laws, in particular for the shallow water equations in 1D and 2D. We focus on the application of monotonicity-preserving interpolatory techniques as a tool for the recursive computation of the numerical divergence in the different grids, which is a key step on multilevel schemes. Numerical tests confirm that this technique leads to a more robust multilevel code while improving its efficiency.

## [01433] Entropy-stable, positivity-preserving and well-balanced Godunov-type schemes for multidimensional shallow-water system

**Format :** Talk at Waseda University

**Author(s) :** Agnès Chan (CEA Cesta - Université de Bordeaux)Gérard Gallice (CEA Cesta)Raphaël Loubère (Université de Bordeaux)Pierre-Henri Maire (CEA Cesta)Alessia Del Grosso (CEA Cesta - Université de Bordeaux)

**Abstract :** An entropy stable, positivity preserving Godunov-type scheme for multidimensional hyperbolic systems of conservation laws on unstructured grids was presented by Gallice et al. in 2022. A specific feature of their Riemann solver is coupling all cells in the vicinity of the current one, making their solver no longer 1D across one edge.

We extend their work to handle source terms, specifically for shallow water equations. The scheme we obtain is well-balanced in 1D and 2D.

## [01511] Numerical solution of a system of conservation laws with discontinuous flux modelling flotation with sedimentation

**Format :** Talk at Waseda University

**Author(s) :** Raimund Bürger (Universidad de Concepción)Stefan Diehl (Lund University)Carmen Martí Raga (Universitat de València)Yolanda Vásquez (Universidad de Concepción)

**Abstract :** Froth flotation is a unit operation used in mineral processing to separate valuable mineral particles from worthless gangue particles in finely ground ores. In this talk, we will present a model for froth flotation, including the drainage of liquid that occurs at the top of the column. We will detail the construction of steady-state solutions and present some results that show the ability of the model to capture steady operation of the flotation device.

**[01508] Implicit and IMEX Lagrange Projection schemes for Ripa model****Format :** Talk at Waseda University**Author(s) :** Celia Caballero Cárdenas (Universidad de Málaga)Manuel Jesús Castro Díaz (Universidad de Málaga)Tomas Morales de Luna (Universidad de Málaga)María Luz Muñoz-Ruiz (Universidad de Málaga)**Abstract :** We consider the one-dimensional system of shallow equations with horizontal temperature gradients, i.e., the Ripa system. We present a numerical approximation of this system based on a Lagrange-Projection type finite volume scheme. We shall consider fully implicit and implicit-explicit versions of the scheme for the Lagrangian step, while the Projection step will always be done explicitly. Several numerical experiments are included in order to illustrate the good behavior of the proposed schemes.

00529 (2/2) : 2C @G606 [Chair: Cipriano Escalante]

**[01400] Vertical discretizations of Euler systems and application to bedload problems****Format :** Talk at Waseda University**Author(s) :** José Garres-Díaz (Universidad de Córdoba)Tomas Morales de Luna (Universidad de Málaga)Cipriano Escalante Sanchez (Universidad de Málaga)Manuel Castro Díaz (Universidad de Málaga)**Abstract :** Shallow water type systems are very popular in numerical simulation of geophysical flows, mainly due to their low computational cost. However, these systems share an important drawback: the vertical information of the flow is lost. In this talk, we present a general framework for vertical discretizations of free-surface Euler system, that generalizes the moment and multilayer techniques. It is called multilayer-moment approach. Several tests are presented, pointing out advantages/disadvantages of each approach, and their efficiency.**[01507] Numerical methods for viscoplastic flows : balancing precision and acceleration****Format :** Talk at Waseda University**Author(s) :** Clément Berger (UMPA CNRS UMR 5669, ENS de Lyon)**Abstract :** We consider here equations for yield stress flows formulated as variational inequalities. The reason is that it allows the best numerical computation of the interfaces between fluid zones and rigid zones. In this talk, we compare multiple optimization methods, from proximal algorithms to second-order cone programming. The compromise between precision and speed differs from one method to another. We will also comment on each associated convergence criteria.**[01504] Digital Twins (DT) on geophysical extreme hazards. Using Tsunami-HySEA numerical model as DT for tsunami hazards.****Format :** Talk at Waseda University**Author(s) :** Jose Manuel Gonzalez-Vida (Dpt. Applied Mathematics. University of Malaga)Jorge Macías (Dpt. Mathematical Analysis, Statistics and Applied Mathematics)Manuel J. Castro (Dpt. Mathematical Analysis, Statistics and Applied Mathematics)Alex González (Dpt. Mathematical Analysis, Statistics and Applied Mathematics)**Abstract :** A Digital Twin (DT) for GEophysical extremes (DT-GEO) is an European project that aims to analyse and forecast the impact of tsunamis, earthquakes, volcanoes, and anthropogenic seismicity. This work address tsunami hazard phenomena to conduct precise data-informed early warning systems, forecasts, and tsunami-hazard assessments across multiple time scales.**[01513] Novel schemes for overdetermined thermodynamically compatible hyperbolic systems****Format :** Online Talk on Zoom**Author(s) :** Saray Busto (Universidade de Vigo)Michael Dumbser (University of Trento)**Abstract :** We introduce a novel efficient general class of thermodynamically compatible, HTC, semi-discrete finite volume and discontinuous Galerkin schemes for overdetermined HTC systems. The approach is based on the discretization of the entropy being the total energy conservation a direct consequence of the HTC discretization. The obtained schemes are provably marginally stable in the energy norm, satisfy a discrete entropy inequality by construction and are assessed using classical benchmarks for turbulent shallow water and compressible flows.

# [00533] Recovery and robustness of geometric fingerprints for point clouds and data

**Session Time & Room :**

00533 (1/3) : 1C (Aug.21, 13:20-15:00) @F412

00533 (2/3) : 1D (Aug.21, 15:30-17:10) @F412

00533 (3/3) : 1E (Aug.21, 17:40-19:20) @F412

**Type :** Proposal of Minisymposium

**Abstract :** The aim of our mini-symposium is to connect communities interested in the problem of condensing information from a dataset to a less complex geometric/statistical "summary", sometimes called a fingerprint. We will concentrate especially on, Distance histograms, Persistence diagrams, as well as spectral fingerprints and other geometric fingerprints. Questions relevant to applications, including topics such as resistance or stability to noise/error of a given fingerprint ("robustness" problems), or injectivity of the fingerprint (relevant for "recovery" problems) will be our focus during the minisymposium.

**Organizer(s) :** Mircea Petrache, Rodolfo Viera

**Classification :** 53C23, 55N31, 68T09, 52C35, 68R12, Distance histograms, Persistence diagrams, Fourier fingerprints

**Minisymposium Program :**

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00533 (1/3) : 1C @F412 [Chair: Petrache Mircea]

## [04178] Recovering discrete Fourier spectra from random perturbations

**Format :** Online Talk on Zoom

**Author(s) :** Mircea Petrache (Pontificia Catolica Universidad de Chile)Rodolfo Viera (Pontificia Universidad Católica de Chile)

**Abstract :** In this talk I will discuss the behaviour of the Fourier Transform of (quasi-)periodic sets under random perturbations. We will see that for i.i.d random perturbations of a quasi-periodic set  $X$  in the Euclidean space, the effect of the perturbations is almost surely that of multiplying the Fourier Transform of  $X$  by a weight which depends on the law of the perturbation. Also we will see quantitative versions of the previous discussion in finite groups which we will use to obtain, after passing to the limit, the almost sure recovery of the Fourier Transform of lattices in some non-abelian instances, such as the Heisenberg group.

## [04956] An information-theoretic perspective on the turnpike and beltway problems

**Format :** Online Talk on Zoom

**Author(s) :** Shuai Huang (Emory University)

**Abstract :** Reconstructing a set of points on a line or a loop from their unlabelled pairwise distances is known as the turnpike or beltway problem. Some point configurations are easy to reconstruct, while others are more difficult. We show that the difficulty of problem can be characterized by the mutual information  $I(X; Y)$  between the point variable  $X$  and distance variable  $Y$ . Experiments show that  $I(X; Y)$  decreases when there are more repeated distances.

## [04313] Curvature sets and curvature measures over persistence diagrams

**Format :** Talk at Waseda University

**Author(s) :** Facundo Memoli (Ohio State University)

**Abstract :** We study an invariant (i.e. a feature) of compact metric spaces which combines the notion of curvature sets introduced by Gromov in the 1980s together with the notion of Vietoris-Rips persistent homology. For given integers  $k \geq 0$  and  $n \geq 1$  these invariants arise by considering the degree  $k$  Vietoris-Rips (VR) persistence diagrams of all finite point clouds with cardinality at most  $n$  sampled from a given metric space. We call these invariants \emph{persistence sets}. This family of invariants contains the usual VR persistence diagram of the original space (when  $n$  is large enough). We argue that for a certain range of values of parameters  $n$  and  $k$ , (1) the family of these invariants 'sees' information not detected by the VR persistence diagrams of the whole space and (2) computing these invariants is significantly easier than computing the usual VR persistence diagrams.

We establish stability results for our persistence sets and also precisely characterize some of them in the case of spheres with geodesic and Euclidean distances. We identify a rich family of metric graphs for which the invariant determined by n=4 and k=1 fully recovers their homotopy type. Along the way we prove some novel properties of VR persistence diagrams.

## [05121] Learning with persistence diagrams

**Format :** Talk at Waseda University

**Author(s) :** Jose Perea (Northeastern University)Iryna Hartsock (University of Florida)Alex Elchesen (Colorado State University)Tatum Rask (Colorado State University)

**Abstract :** Persistence diagrams are common descriptors of the topological structure of data appearing in various classification and regression tasks. They can be generalized to Radon measures supported on the birth-death plane and endowed with an optimal transport distance. Examples of such measures are expectations of probability distributions on the space of persistence diagrams. In this talk, I will present methods for approximating continuous functions on the space of Radon measures supported on the birth-death plane, as well as their utilization in supervised learning tasks.

00533 (2/3) : 1D @F412 [Chair: Petrache Mircea]

## [04676] Persistent cycle registration and topological bootstrap

**Format :** Online Talk on Zoom

**Author(s) :** Yohai Reani (Viterbi Faculty of Electrical Engineering, Technion - Israel Institute of Technology)Omer Bobrowski (Viterbi Faculty of Electrical Engineering, Technion - Israel Institute of Technology)

**Abstract :** In this talk we present a novel approach for comparing the persistent homology representations of two spaces (filtrations) directly in the data space. We do so by defining a correspondence relation between such representations and devising a method, based on persistent homology variants, for its efficient computation. We demonstrate our new framework in the context of topological inference, where we use statistical bootstrap-like methods to differentiate between real phenomena and "noise" in point cloud data.

## [05127] The Density Fingerprint of a Periodic Set and Persistent Homology

**Format :** Online Talk on Zoom

**Author(s) :** Herbert Edelsbrunner (Institute of Science and Technology Austria)Teresa Heiss (Institute of Science and Technology Austria)Vitaliy Kurlin (University of Liverpool)Philip Smith (University of Liverpool)Mathijs Wintraecken (Institute of Science and Technology Austria)

**Abstract :** Modeling a crystal as a periodic point set, we present a fingerprint consisting of density functions. The density fingerprint is invariant under isometries, continuous, and complete in the generic case, which are necessary features for reliable comparison of crystals. The fingerprint has a fast algorithm based on Brillouin zones and related inclusion-exclusion formulae, which we have implemented. I will discuss the connection with persistent homology, suggesting a possible extension of the fingerprint.

## [04866] Reconstruction of manifolds from point clouds and inverse problems

**Format :** Talk at Waseda University

**Author(s) :** Matti Lassas (University of Helsinki)Charles Fefferman (Princeton University)Sergei Ivanov (Steklov Institute of Mathematics)Hariharan Narayanan (Tata Institute for Fundamental Research)Jinpeng Lu (University of Helsinki)

**Abstract :** We consider a geometric problem on how a Riemannian manifold can be constructed to approximate a given discrete metric space. This problem is closely related to invariant manifold learning, where a Riemannian manifold  $(M, g)$  needs to be approximately constructed from the noisy distances  $d(X_j, X_k) + \eta_{jk}$  of points  $X_1, X_2, \dots, X_N$ , sampled from the manifold  $M$ . Here,  $d(X_j, X_k)$  are the distance of the points  $X_j, X_k \in M$  and  $\eta_{jk}$  are random measurement errors. The values  $d(X_j, X_k)$  can be considered as distance fingerprints of the manifold  $M$ .

We also consider applications of the results in inverse problems encountered in medical and seismic imaging. In these problems, an unknown wave speed in a domain needs to be determined from indirect measurements. Moreover, we discuss a problem analogous to the above one, where distances are measured from points in a small subset  $U \subset M$  to points in a discrete subset of  $M$  and the errors are deterministic.

00533 (3/3) : 1E @F412

# [00534] Topological and geometric data analysis: theory and applications

**Session Time & Room :**

00534 (1/2) : 2C (Aug.22, 13:20-15:00) @F412

00534 (2/2) : 2D (Aug.22, 15:30-17:10) @F412

**Type :** Proposal of Minisymposium

**Abstract :** In recent decades, topological data analysis "TDA" and geometric data analysis "GDA" have provided great impacts on data science, characterizing valuable information on "shape of data". In this series of mini-symposia, we present recent progresses of theory and applications of TDA and GDA, including persistent homology, optimal transportation, filling radius, Reeb graph, graph embeddings, flow data analysis, dimensionality reduction, geometric deep learning, Hodge Laplacian, discrete exterior calculus, and their various applications in materials, chemistry, biology, and data sciences.

**Organizer(s) :** Yasuaki Hiraoka, Kelin Xia

**Classification :** 55N31, 62R40

**Minisymposium Program :**

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00534 (1/2) : 2C @F412 [Chair: Yasuaki Hiraoka]

## [01514] Vietoris-Rips persistent homology, injective metric spaces, and the filling radius

**Format :** Talk at Waseda University

**Author(s) :** Sunhyuk Lim (Max Planck Institute for Mathematics in the Sciences)Facundo Memoli (The Ohio State University)Osman Berat Okutan (Florida State University)

**Abstract :** In the applied algebraic topology community, the persistent homology induced by the Vietoris-Rips simplicial filtration is a standard method for capturing topological information from metric spaces. In this paper, we consider a different, more geometric way of generating persistent homology of metric spaces which arises by first embedding a given metric space into a larger space and then considering thickenings of the original space inside this ambient metric space. In the course of doing this, we construct an appropriate category for studying this notion of persistent homology and show that, in a category theoretic sense, the standard persistent homology of the Vietoris-Rips filtration is isomorphic to our geometric persistent homology provided that the ambient metric space satisfies a property called injectivity.

As an application of this isomorphism result we are able to precisely characterize the type of intervals that appear in the persistence barcodes of the Vietoris-Rips filtration of any compact metric space and also to give succinct proofs of the characterization of the persistent homology of products and metric gluings of metric spaces. Our results also permit proving several bounds on the length of intervals in the Vietoris-Rips barcode by other metric invariants, for example the notion of spread introduced by M. Katz.

As another application, we connect this geometric persistent homology to the notion of filling radius of manifolds introduced by Gromov and show some consequences related to (1) the homotopy type of the Vietoris-Rips complexes of spheres which follow from work of M. Katz and (2) characterization (rigidity) results for spheres in terms of their Vietoris-Rips persistence barcodes which follow from work of F. Wilhelm.

Finally, we establish a sharp version of Hausmann's theorem for spheres which may be of independent interest.

## [01746] Reeb Order Method and its Application to Topological Flow Data Analysis

**Format :** Talk at Waseda University

**Author(s) :** Tomoki UDA (Tohoku University)

**Abstract :** Sakajo and Yokoyama have classified the topology of streamlines and characterised them by unique tree representations, called Cyclically Ordered rooted Tree (COT) representations. The author realised the practical application of their theory to data science, called Topological Flow Data Analysis (TFDA), utilising Reeb graphs and their discretised version, Reeb order. In this talk, we briefly introduce TFDA theory and its application to meteorology and oceanography.

## [04575] Topological Node2vec: Graph Embeddings via Persistent Homology

**Format :** Talk at Waseda University

**Author(s) :** Killian Meehan (Kyoto University)

**Abstract :** Node2vec is a machine learning framework which specializes in transforming graph into euclidean data. However, we demonstrate that with very simple examples we see a high destruction of topological information during the embedding process. Our project builds on top of the original Node2vec framework and introduces a topological loss function derived from optimal transport which forces this new machine learning network to maximally preserve graph information while checking topological loss at every step.

## [04694] Data, Geometry, and homology

**Format :** Talk at Waseda University

**Author(s) :** Wojciech Chacholski (KTH, Royal Institute of Technology)Jens Agerberg (KTH, Royal Institute of Technology and Ericsson)Ryan Ramanujam (Karolinska Institutet (Dept. of Clinical Neuroscience) and Datanon Corporation)Francesca Tombari (KTH, Royal Institute of Technology)

**Abstract :** For a successful analysis a suitable representation of data by objects amenable for statistical methods is fundamental.

There has been an explosion of applications in which homological representations of data played a significant role. I will present one such representation called stable rank and introduce various novel ways of using it to encode geometry, and then analyse, data. I will provide several illustrative examples of how to use stable ranks to find meaningful results.

00534 (2/2) : 2D @F412 [Chair: Kelin Xia]

## [04865] Topological Representation Learning for Biomedical Image Analysis

**Format :** Talk at Waseda University

**Author(s) :** Chao Chen (Stony Brook University)

**Abstract :** Modern analytics is facing highly complex and heterogeneous data. While deep learning models have pushed our prediction power to a new level, they are not satisfactory in some crucial merits such as transparency, robustness, data-efficiency, etc. In this talk, I will focus on our recent work on combining topological reasoning with learning to solve problems in biomedical image analysis. In biomedicine, we encounter various complex structures such as neurons, vessels, tissues and cells. These structures encode important information about underlying biological mechanisms. To fully exploit these structures, we propose to enhance learning pipelines through the application of persistent homology theory. This inspires a series of novel methods for segmentation, generation, and analysis of these topology-rich biomedical structures. Complex structures also arise in many other contexts beyond biomedicine. We will also briefly introduce how topological reasoning can be used to strengthen graph neural networks and to improve the robustness of deep neural networks against noise and against backdoor attacks.

## [05110] New Algorithms for Random Graph Embeddings

**Format :** Talk at Waseda University

**Author(s) :** Jason H Cantarella (University of Georgia)Clayton Shonkwiler (Colorado State University)Henrik Schumacher (Technische Universität Chemnitz)Tetsuo Deguchi (Ochanomizu University)Erica Uehara (Kyoto University)

**Abstract :** We discuss the problem of randomly embedding graphs in  $R^d$ , which often arises in machine learning. Given an arbitrary probability distribution on each edge, we condition the joint distribution on the graph type (loops of edges must close). The key idea is to use an unusual version of cohomology to encode embedding data. Our method is particularly well suited to embeddings with fixed edge lengths, which arise in polymer science and robotics.

## [05318] Topological Deep Learning: Going Beyond Graph Data

**Format :** Talk at Waseda University

**Author(s) :** Mustafa Hajij (University of San Francisco)Ghada Zamzmi (University of South Florida)Theodore Papamarkou (University of Manchester)Nina Miolane (University of California Santa Barbara)Aldo Saenz (IBM)Karthikeyan Natesan Ramamurthy (IBM)Tolga Birdal (Imperial College London)Tamal Krishna Dey (Purdue University)Soham Mukherjee (Purdue University)Shreyas Samaga (Purdue University)Neal Livesay (Northeastern University)Robin Walters (Northeastern University)Paul Rosen (University of Utah)Michael Schaub (RWTH Aachen University)

**Abstract :** Topological deep learning is a rapidly growing field that pertains to the development of deep learning models for data supported on topological domains such as simplicial complexes, cell complexes, and hypergraphs, which generalize many domains encountered in scientific computations. In this paper, we present a unifying deep learning framework built upon a richer data structure that includes widely adopted topological domains.

Specifically, we first introduce combinatorial complexes, a novel type of topological domain. Combinatorial complexes

can be seen as generalizations of graphs that maintain certain desirable properties. Similar to hypergraphs, combinatorial complexes impose no constraints on the set of relations. In addition, combinatorial complexes permit the construction of hierarchical higher-order relations, analogous to those found in simplicial and cell complexes. Thus, combinatorial complexes generalize and combine useful traits of both hypergraphs and cell complexes, which have emerged as two promising abstractions that facilitate the generalization of graph neural networks to topological spaces.

Second, building upon combinatorial complexes and their rich combinatorial and algebraic structure, we develop a general class of message-passing combinatorial complex neural networks (CCNNs), focusing primarily on attention-based CCNNs. We characterize permutation and orientation equivariances of CCNNs, and discuss pooling and unpooling operations within CCNNs in detail.

Third, we evaluate the performance of CCNNs on tasks related to mesh shape analysis and graph learning. Our experiments demonstrate that CCNNs have competitive performance as compared to state-of-the-art deep learning models specifically tailored to the same tasks. Our findings demonstrate the advantages of incorporating higher-order relations into deep learning models in different applications.

## [01521] Topological approaches to higher-order interaction networks

**Format :** Online Talk on Zoom

**Author(s) :** Jie Wu Wu (Yanqi Lake Beijing Institute of Mathematical Sciences and Applications (BIMSA))

**Abstract :** In this talk, guided by the applications to higher-order interaction network, we will discuss some topological approaches to graphs and hypergraphs beyond TDA, including GLMY homology of digraphs introduced by S. T. Yau et al, and their generalizations such as embeded homology of hypergraphs, which is an extension of simplicial homology. We will also report some of our recent works on the topic, including a frame work for introducing a new theory which unifies various aspects of topological approaches for data science, by being applicable both to point cloud data and to graph datas.

## [00538] Mathematical modeling, analysis, and simulation for complex neural systems

**Session Time & Room :**

00538 (1/2) : 5C (Aug.25, 13:20-15:00) @A511

00538 (2/2) : 5D (Aug.25, 15:30-17:10) @A511

**Type :** Proposal of Minisymposium

**Abstract :** Mathematical neuroscience exploits applied mathematics tools, e.g., modeling, analysis and scientific computing, to understand the structure, dynamics, and function of the brain. Many neuroscience phenomena are intriguing but extremely complicated, with features of high dimensionality, nonlinearity, multi-scale, and complex dynamics. Therefore, developing effective theoretical and computational methods becomes increasingly significant to understand the mechanism underlying neuroscience phenomena, as well as to advance experimental neuroscience. This mini-symposium focuses on novel ideas and advanced approaches in mathematical neuroscience, with an emphasis on prominent neuroscience phenomena including hierarchical structure, oscillatory and attractor dynamics, and functions of learning and memory.

**Organizer(s) :** Songting Li, Douglas Zhou

**Classification :** 92-10, 37Nxx, 62Pxx

**Minisymposium Program :**

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00538 (1/2) : 5C @A511 [Chair: Songting Li]

## [04042] Learning optimal models of statistical events in spontaneous neural activity

**Format :** Talk at Waseda University

**Author(s) :** Toshitake Asabuki (Imperial College London) Tomoki Fukai (Okinawa Institute of Science and Technology)

**Abstract :** The brain is thought to learn an internal model of the statistical environment for improved cognitive performance. Evidence suggests that spontaneous cortical activity represents such a model, or prior distribution, by replaying stimulus-evoked activity patterns with the probabilities that these stimuli were experienced. Here, we present a principle to robustly learn replay activity patterns in spiking recurrent neural networks and demonstrate how such spontaneous replay biases animals' perceptual decision making.

**[03841] The hierarchical organization of the Drosophila connectome****Format :** Talk at Waseda University**Author(s) :** Kresimir Josic (University of Houston) Alexander B. Kunin (Creighton University) Jiahao Guo (University of Houston) Kevin E. Bassler (University of Houston) Xaq Pitkow (Rice University)**Abstract :** The Hemibrain is the largest published connectome to date. It is the result of a dense reconstruction of over twenty thousand neurons and ten million synapses spanning the fruit fly Drosophila central brain. I will describe a novel approach to uncovering the hierarchical community structure of this connectome. This approach allows us to recover previously known and reveal novel features of the organization within the fly brain. Methods such as these will be essential to interpret the forthcoming connectomics data due to its size and complexity.**[01437] The mechanism of abnormal beta-oscillation generated in striatum****Format :** Talk at Waseda University**Author(s) :** Douglas Zhou (Shanghai Jiao Tong University)**Abstract :** combining simulations of a neural network model and the analysis of the corresponding reduced neural mass model, we demonstrate how the cellular architecture and network dynamics of the ChAT - iMSN close loop in the striatum efficiently yield exaggerated beta oscillations. We find that beta oscillations can emerge from inhibitory interactions among iMSNs. And a slow inhibitory dynamic in iMSNs could be the underpinning of beta oscillations.**[03947] Maturation of neurons reconciles flexibility and stability of memory: dual structural plasticity in the olfactory system****Format :** Talk at Waseda University**Author(s) :** Bennet Sakelaris (Northwestern University) Hermann Riecke (Northwestern University)**Abstract :** It is essential for the brain to flexibly form new memories without overwriting and jeopardizing the stability of existing ones. Using a computational model of the olfactory bulb (OB) that captures several experimental observations, we investigate how the characteristic structural plasticity of the OB addresses this flexibility-stability tradeoff. We demonstrate that the evolution of the timescales of synaptic plasticity associated with the aging of adult-born cells allows the OB to strike a harmonious balance between the competing demands of flexibility and stability.

00538 (2/2) : 5D @A511 [Chair: Douglas Zhou]

**[01409] Mathematical mechanism underlying hierarchical timescales in the primate neocortex****Format :** Talk at Waseda University**Author(s) :** Songting Li (Shanghai Jiao Tong University)**Abstract :** In the neocortex, while early sensory areas encode and process external inputs rapidly, higher-association areas are endowed with slow dynamics to benefit information accumulation over time. Such a hierarchy of temporal response windows along the cortical hierarchy naturally emerges in an anatomically based model of primate cortex. The emergent property raises the question of why diverse temporal modes are well segregated rather than being mixed up across the cortex, despite high connection density and an abundance of feedback loops. In this talk, we will address this question by mathematically analyzing the primate cortical model and identifying crucial conditions of synaptic excitation and inhibition that give rise to timescale segregation in a hierarchy. In addition, we will discuss the mathematical relation between timescales segregation and signal propagation in the cortex.**[04184] Computation with Adaptive Continuous Attractor Neural Networks****Format :** Online Talk on Zoom**Author(s) :** SI WU (Peking University)**Abstract :** Continuous attractor neural networks (CANNs) are a canonical model for neural information representation, storing, retrieving and manipulation. Adaptation is a general feature of neural systems referring to a negative feedback process when neuronal activity is high. When two of them are combined together, the neural network exhibits rich dynamical behaviors. In this talk, I will introduce the rich dynamical properties of adaptive CANNs and their potential roles in brain functions.

## [03884] Learning biological neuronal networks with artificial neural networks: Neural oscillations

**Format :** Online Talk on Zoom

**Author(s) :** Louis Tao (Peking University)Ruilin Zhang (Peking University)Zhongyi Wang (Peking University)Tianyi Wu (New York University)Yuhang Cai (University of California at Berkeley)Zhuo-cheng Xiao (New York University)Yao Li (University of Massachusetts)

**Abstract :** First-principles-based models have been extremely successful in providing crucial insights and predictions for complex biological functions and phenomena. However, they can be hard to build and expensive to simulate for complex living systems. On the other hand, modern data-driven methods thrive at modeling many types of high-dimensional and noisy data. Still, the training and interpretation of these data-driven models remain challenging. Here, we combine the two types of methods to model stochastic neuronal network oscillations. Specifically, we develop a class of first-principles-based artificial neural networks to provide faithful surrogates to the high-dimensional, nonlinear oscillatory dynamics produced by neural circuits in the brain. Furthermore, when the training data set is enlarged within a range of parameter choices, the artificial neural networks become generalizable to these parameters, covering cases in distinctly different dynamical regimes. In all, our work opens a new avenue for modeling complex neuronal network dynamics with artificial neural networks.

## [01458] Reconstruction of Evolving Percepts in Binocular Rivalry Using Novel Model Network Dynamics

**Format :** Online Talk on Zoom

**Author(s) :** Victor Barranca (Swarthmore College)

**Abstract :** When the two eyes are presented with distinct stimuli, our percept irregularly switches between the monocular images, giving rise to binocular rivalry. We investigate mechanisms for rivalry through stimulus reconstructions based on the activity of a two-layer neuronal network model with competing downstream pools driven by disparate monocular images. To estimate the dynamic percept, we derive an embedded input-output mapping and iteratively apply compressive sensing techniques, generating percept reconstructions that agree with key experimental observations.

## [00539] Extreme value theory and statistical analysis

**Session Time & Room :** 4D (Aug.24, 15:30-17:10) @F412

**Type :** Proposal of Minisymposium

**Abstract :** Huge disasters, such as earthquake and flood occur rarely but their damage is extremely terrible and the countermeasures against them are urgent social task.

Extreme value theory (EVT) deals with rare events mathematically or statistically and is applied to risk management for not only disasters but also various fields, for example, finance, insurance and life span of industrial products.

We present 4 researches. Asymptotic theory for extreme value generalized additive model, statistical inference for sample maximum distribution, nonparametric statistical inference related to several economic topics and statistical management for multivariate risk for financial institutions.

**Organizer(s) :** Takaaki SHIMURA

**Classification :** 60G70, 62G32, 62E20, 62G08, 62H05

**Minisymposium Program :**

00539 (1/1) : 4D @F412 [Chair: Takuma Yoshida]

## [03480] Asymptotic theory for extreme value generalized additive model

**Format :** Talk at Waseda University

**Author(s) :** Takuma Yoshida (Kagoshima University)

**Abstract :** The classical approach to analyzing extreme value data is the generalized Pareto distribution (GPD). When the GPD is used to explain a target variable with the large dimension of covariates, the shape and scale function of covariates included in GPD are sometimes modeled using the generalized additive models (GAM). In contrast to many results of application, there are no theoretical results on the hybrid technique of GAM and GPD, which motivates us to develop its asymptotic theory. We provide the rate of convergence of the estimator of shape and scale functions, as well as its local asymptotic normality.

## [03597] Comparative study on accuracy of sample maximum distribution estimators in IID settings

**Format :** Online Talk on Zoom

**Author(s) :** Taku Moriyama (Yokohama City University)

**Abstract :** Comparative study on the accuracy of sample maximum distribution estimators in IID settings will be reported. The distribution of sample maximum is approximated by the generalized extreme value distribution. However, the approximation accuracy heavily depends on the tail index. This study investigates a nonparametric estimator as the alternative approach and compares the accuracies both theoretically and numerically. Future prospects of the study will also be discussed.

## [02777] Subsampling inference for nonparametric extremal conditional quantiles

**Format :** Talk at Waseda University

**Author(s) :** Daisuke Kurisu (The University of Tokyo)Taisuke Otsu (London School of Economics)

**Abstract :** In this talk, we study asymptotic properties of the local linear (LL) quantile estimator under the extremal-order quantile asymptotics and develop a practical inference method for conditional quantiles in extreme tail areas. The asymptotic distribution of the LL quantile estimator is derived as a minimizer of certain functional of a Poisson point process. We also propose a subsampling inference method for conditional extreme quantiles based on a self-normalized version of the LL estimator.

## [03093] Measuring non-exchangeable tail dependence using tail copulas

**Format :** Talk at Waseda University

**Author(s) :** Takaaki Koike (Hitotsubashi University)Shogo Kato (Institute of Statistical Mathematics)Marius Hofert (The University of Hong Kong)

**Abstract :** We propose a novel framework of quantifying and comparing the degree of tail dependence using tail copula. Our proposed measures have clear probabilistic interpretations, and capture various features of non-exchangeable tail dependence depending on the purpose of the analysis. Analytical forms of the proposed measures are derived for various parametric copulas. A real data analysis reveals striking tail dependence and tail non-exchangeability of the return series of stock indices, particularly in periods of financial distress.

## [00545] Waves in complex and multiscale media

**Session Time & Room :**

00545 (1/3) : 5B (Aug.25, 10:40-12:20) @G406

00545 (2/3) : 5C (Aug.25, 13:20-15:00) @G406

00545 (3/3) : 5D (Aug.25, 15:30-17:10) @G406

**Type :** Proposal of Minisymposium

**Abstract :** Characterizing wave propagation in complex and multiple-scale media is important for modelling and simulating the propagation of acoustic, electromagnetic, elastic and water waves in heterogeneous media. This minisymposium demonstrates the ubiquity of mathematical techniques by bringing together researchers from all of these application areas. The talks will illustrate a variety of the current methods and the challenges that remain. The session will represent a cross section of applied mathematics, ranging from applied analysis to large-scale numerical simulation schemes. A central aim of the minisymposium is to promote the exchange of ideas and knowledge between the different application areas.

**Organizer(s) :** Bryn Davies, Luke Bennetts

**Classification :** 35J05, 76B15, 34M30

**Minisymposium Program :**

00545 (1/3) : 5B @G406 [Chair: Bryn Davies]

## [03757] Effective waves in random particulate media: introduction and numerical validation

**Format :** Talk at Waseda University

**Author(s) :** ARTUR LEWIS GOWER (University of Sheffield)Stuart Hawkins (Macquarie University)Gerhard Kristensson (Lund University)

**Abstract :** Describing how waves scattering between a large set of particles is challenging. There are accurate numerical methods, but they lack intuition and can be slow. Effective theory is a method to replace the particles with a homogeneous media which leads to greater intuition and is quick to calculate. One drawback is often that effective theory is only accurate for long wavelengths. In this talk, I will show how we overcame the challenges to extend effective theory for a large range of wavelengths ( $0 < k a < 2$ ) and material properties (particle type and volume fractions) for waves in a random particulate material.

## [04234] Scattered wavefield in the stochastic homogenization regime

**Format :** Talk at Waseda University

**Author(s) :** Laure Giovangigli (ENSTA Paris)Quentin Goepfert (ENSTA Paris)Pierre Millien (Institut Langevin, ESPCI)Josselin Garnier (Ecole Polytechnique)

**Abstract :** This work aims at modelling and studying the propagation and diffusion of ultrasounds in complex multi-scale media such as biological tissues or composite materials. We consider in the free space a homogeneous bounded medium in which lie randomly distributed inhomogeneities that are small compared to the wavelength. In order to characterize the response of this medium to an incident plane wave, we perform an asymptotic expansion of the scattered wave with respect to the size of the inhomogeneities using stochastic homogenisation techniques. The difficulties lie in the transmission conditions at the boundary of the medium. We derive quantitative error estimates given that the random distribution of inhomogeneities verifies mixing properties. Finally we present numerical simulations to illustrate and validate our results.

## [04262] Waves on Graphs

**Format :** Talk at Waseda University

**Author(s) :** Gregor Tanner (University of Nottingham)Stephen C Creagh (University of Nottingham)Cerian Brewer (University of Nottingham)

**Abstract :** We consider the wave dynamics on networks or graphs carrying both propagating and evanescent modes on each edge. This is an extension of quantum graph theory and occurs naturally when considering networks of plates or beams with different mode types (flexural, longitudinal and shear waves) propagating on each connecting structure. The local vertex scattering matrices and the global transfer operator are no longer unitary with interesting consequences for secular equations and the Weyl law.

## [04615] Designing large-scale acoustic scattering systems using structural optimization and multiple scattering theory

**Format :** Talk at Waseda University

**Author(s) :** Kei Matsushima (The University of Tokyo)Takayuki Yamada (The University of Tokyo)

**Abstract :** In this talk, we present a numerical scheme for designing large-scale acoustic scattering systems based on a multiple scattering theory and shape/topology optimization. We first solve exterior Helmholtz problems using the T-matrix method. This formulation allows us to evaluate a design sensitivity of multiple scattering systems using the adjoint variable method. We will demonstrate that the proposed scheme can design an omnidirectional acoustic cloak.

00545 (2/3) : 5C @G406 [Chair: Luke Bennetts]

## [04940] Bounds on the Quality-factor of Two-phase Quasi-static Metamaterial Resonators and Optimal Microstructure Designs

**Format :** Talk at Waseda University

**Author(s) :** Kshiteej Deshmukh (University of Utah)Graeme Milton (University of Utah)

**Abstract :** Material resonances are fundamentally important in the field of nano-photonics and optics. So it is of great interest to

know what are the limits to which they can be tuned. The bandwidth of the resonances in materials is an important feature which is commonly characterized by using the quality (Q) factor. We present bounds on the quality factor of two-phase quasi-static metamaterial resonators evaluated at a given resonant frequency by introducing an alternative definition for the Q-factor in terms of the complex effective permittivity of the composite material. Optimal metamaterial microstructure designs achieving points on these bounds are presented. The most interesting optimal microstructure, is a limiting case of doubly coated ellipsoids, consisting of a dilute suspension of ellipsoids near resonance

sandwiched between layers. It attains points on the lower bound for the Q-factor. We also obtain bounds on Q for three dimensional, isotropic, and fixed volume fraction two-phase quasi-static metamaterials. Some almost optimal isotropic microstructure geometries are identified.

## [04245] Band structure and Dirac points of real-space quantum optics in periodic media

**Format :** Talk at Waseda University

**Author(s) :** Erik Orvehed Hiltunen (Yale University)John Schotland (Yale University)Michael Weinstein (Columbia University)Joseph Kraisler (Columbia University)

**Abstract :** The field of photonic crystals is almost exclusively based on a Maxwell model of light. While often an effective model, it is natural to study such systems under a quantum-mechanical photon model instead. In the real-space parametrization, interacting photon-atom systems are governed by a system of \emph{nonlocal} partial differential equations. In this talk, we study resonant phenomena of such systems. Using integral equations, we phrase the resonant problem as a nonlinear eigenvalue problem. In a setting of high-contrast atom inclusions, we obtain fully explicit characterizations of resonances, band structure, and Dirac cones. Additionally, we present a strikingly simple relation between the Green's function of the nonlocal equation and that of the local (Helmholtz) equation. Based on this, we are able to achieve highly efficient numerical calculations of band structures of interacting photon-atom systems.

## [03889] Mathematics of in-gap interface modes in photonic/phononic structures in one dimension

**Format :** Talk at Waseda University

**Author(s) :** Hai Zhang (HKUST)Junshan Lin (Auburn University)

**Abstract :** The developments of topological insulators have provided a new avenue for creating interface modes (or edge modes) in photonic/phononic structures. Such created modes have the distinct property of being topologically protected and are stable with respect to perturbations in certain classes. In this talk, we will report recent results on the existence of an in-gap interface mode that is bifurcated from a Dirac point in a photonic/phononic structure in one dimension.

## [04807] Recent advances in the theory of field patterns

**Format :** Talk at Waseda University

**Author(s) :** Ornella Mattei (San Francisco State University)Vincenzo Gulizzi (University of Palermo)

**Abstract :** Field pattern materials are spatial composites whose properties are modulated in time in such a way that disturbances propagate along locally periodic networks of characteristic lines, called field patterns. Depending on the material properties, modes can be propagating or can blow up (decay) in time. Here we show how to design the spatial geometry of one- and two-dimensional field pattern materials, so that modes are always stable.

00545 (3/3) : 5D @G406 [Chair: Bryn Davies]

## [05192] Water wave resonances between floating vessels: fundamentals to applications

**Format :** Talk at Waseda University

**Author(s) :** Hugh Wolgamot (University of Western Australia)Wenhua Zhao (University of Western Australia)

**Abstract :** The narrow gap formed between floating vessels in close proximity supports resonances. This leads to a variety of problems of both theoretical and practical interest. In this talk the resonant structure of the coupled motion of the vessels and fluid is first investigated using linear potential flow theory for simple geometries. The interaction of prismatic vessels spanning a channel (a common experimental set-up) is then considered. Interaction with practical mechanical constraints (mooring) is discussed.

## [03152] Broadband energy capture by an array of heaving buoys

**Format :** Talk at Waseda University

**Author(s) :** Amy-Rose Westcott (The University of Adelaide)Luke Bennetts (The University of Adelaide)Benjamin Cazzolato (The University of Adelaide)Nataliia Sergienko (The University of Adelaide)

**Abstract :** Broadband energy capture is sought by grading the resonant properties of an array of heaving buoy-type wave energy converters (WECs) in 2D. Linear potential-flow theory is applied and WEC interactions are modelled using multiple-wave scattering theory. The resonant properties of WECs are tuned via a linear spring-damper power take-off mechanism to manipulate the complex-frequency zeros. The resulting graded array captures near-perfect absorption (>97% of incident energy) from a targeted band of wavelengths spanning 1.5 times the array's length.

## [04111] Graded arrays for spatial frequency separation and amplification of water waves

**Format :** Talk at Waseda University

**Author(s) :** Malte A Peter (University of Augsburg)Luke G Bennetts (University of Adelaide)Richard V Craster (Imperial College London)

**Abstract :** Wave-energy converters extracting energy from ocean waves are known to suffer from poor efficiency. We propose structures substantially amplifying water waves over a broad range of frequencies at selected locations, with the idea of enhanced energy extraction. Using linear potential-flow theory, it is shown that the energy carried by a plane incident wave is amplified within specified locations. Transfer-matrix analysis is used for the analysis and results from wave-flume experiments confirm the amplification in practice.

## [00550] Multi-scale analysis in random media and applications

**Session Time & Room :**

00550 (1/3) : 1E (Aug.21, 17:40-19:20) @G502

00550 (2/3) : 2C (Aug.22, 13:20-15:00) @G502

00550 (3/3) : 2D (Aug.22, 15:30-17:10) @G502

**Type :** Proposal of Minisymposium

**Abstract :** A rich variety of models in mechanics are heterogenous and multi-scale in nature, and the derivation of „averaged“ or „effective“ behaviours on large-scales are well-known to be challenging and of particular interest. The complexity of the micro-structure often requires stochastic modeling and advanced methods, combining tools from PDE and probability, to understand and compute such effective properties. The purpose of this mini-symposium is to offer an overview of recent developments on the theory of stochastic homogenization and its applications in several areas of applied mathematics, ranging from fluids mechanics, wave propagation, nonlinear elasticity and statistical mechanics.

**Organizer(s) :** Nicolas Clozeau, Laure Giovangigli, Lihan Wang

**Classification :** 35Bxx, 74Qxx, 76M50, 35Axx, 82B44

**Minisymposium Program :**

00550 (1/3) : 1E @G502 [Chair: Laure Giovangigli]

## [04699] Recent advances in quantitative stochastic homogenisation of nonlinear models

**Format :** Talk at Waseda University

**Author(s) :** Nicolas Clozeau (Institute of science and technology Austria)Antoine Gloria (Sorbonne Université)Mathias Schäffner (Uni Halle)Julian Fischer (Institute of science and technology Austria)Antonio Agresti (Institute of science and technology Austria)

**Abstract :** I will present recent advances on the quantitative homogenisation of stochastic nonlinear models. First, I will discuss

the case of convex variational models described by its Euler-Lagrange equation, taking the form of a nonlinear elliptic equation in divergence form with monotone and random coefficients. I will present the quantitative homogenisation theory in current development with Antoine Gloria and Mathias Schäffner, aiming at describing the oscillations and fluctuations of solutions at the microscopic scale as well as the large-scale regularity theory of the random nonlinear operator. Second, I will discuss the case of non-convex variational models of Griffith type in fracture mechanics and a quantitative result concerning the convergence of the cell formula recently obtained in collaboration with Julian Fischer and Antonio Agresti.

## [04559] Quantitative Homogenization for Nondivergence Form Equations

**Format :** Talk at Waseda University

**Author(s) :** Jessica Lin (McGill University)

**Abstract :** In this talk, I will first give an overview of stochastic homogenization for nondivergence form equations (from the PDE perspective) and quenched invariance principles for nonreversible diffusion processes (from the probability perspective). I will then present various quantitative stochastic homogenization results and discuss challenges specific to the homogenization of nondivergence form equations. This talk is based on joint work with Scott Armstrong (NYU) and Benjamin Fehrman (Oxford).

## [04584] Quantitative homogenization of elliptic system with periodic and high contrast coefficients

**Format :** Talk at Waseda University

**Author(s) :** Wenjia Jing (Tsinghua University)Xin Fu (Tsinghua University)

**Abstract :** We present several results about the quantitative estimates of the homogenization of elliptic systems in high contrast periodic media. The periodically distributed high contrast parts have physical parameters that are either extremely large or extremely small compared to those in the background. We develop a method that is somewhat unified and can treat both types of high contrast limits. We obtain quantitative convergence rates with proper correctors, uniform Lipschitz regularity for the solutions of the heterogeneous equations and, as an application, a quantitative description of the spectral convergence for the double-porosity problem. We also discuss possible extensions of the method to some other systems, e.g., linear elasticity, with richer high contrast structures.

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00550 (2/3) : 2C @G502 [Chair: Nicolas Clozeau]

## [05476] On the lower spectrum of heterogeneous acoustic operators

**Format :** Online Talk on Zoom

**Author(s) :** Mitia Duerinckx (Université Libre de Bruxelles)

**Abstract :** In this talk, we describe a quantitative link between homogenization and Anderson localization for heterogeneous acoustic operators: we draw consequences on the spatial spreading of eigenstates in the lower spectrum (if any) from the long-time homogenization of the wave equation, through dispersive estimates. This yields an alternative proof (avoiding Floquet theory) that the lower spectrum of the acoustic operator is purely absolutely continuous in case of periodic coefficients, and it further provides nontrivial quantitative lower bounds on the spatial spreading of potential eigenstates in case of quasiperiodic and random coefficients. This is based on joint work with Antoine Gloria.

## [03179] Boundary effects in radiative transfer of acoustic waves in a randomly-fluctuating medium delimited by boundaries

**Format :** Talk at Waseda University

**Author(s) :** Adel Messaoudi (Aix-Marseille université)Régis Cottreau (CNRS)Christophe Gomez (Aix-Marseille université)

**Abstract :** This presentation discusses the derivation of radiative transfer equations for acoustic waves propagating in a randomly-fluctuating half-space and slab in the weak-scattering regime, and the study of boundary effects. These radiative transfer equations allow to model the transport of wave energy density, taking into account the scattering by random heterogeneities. The approach builds on an asymptotic analysis of the Wigner transform of the wave solution and the method of images.

## [05197] Bloch analysis extended to weakly disordered periodic media

**Format :** Online Talk on Zoom

**Author(s) :** Régis Cottreau (CNRS)Yilun Li (CentraleSupélec)Bing Tie (CNRS)

**Abstract :** The dispersion properties of periodic metamaterials can be tailored in order to obtain desirable effects, for instance band gaps over chosen frequency ranges. However, these patterns are sometimes completely destroyed by the small (random) defects introduced by the manufacturing processes, and the induced loss of periodicity of the metamaterials. This contribution explores the extension of the classical Bloch-Floquet theory to problems that are weakly non-periodic, using asymptotic analysis and a random mapping of the properties to a periodic reference.

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00550 (3/3) : 2D @G502 [Chair: Nicolas Clozeau]

## [04385] Gamma-convergence and stochastic homogenisation for phase-transition models

**Format :** Talk at Waseda University

**Author(s) :** Roberta Marziani (TU Dortmund)

**Abstract :** In this talk we discuss the gamma-convergence of general phase-transition functionals of Modica-Mortola type whose integrands depend both on the space variable and on the regularization parameter (which represents the characteristic length scale of phase transition). In particular we show that the limit is a surface functional whose integrand is characterized by the limit of a suitable cell formula. We then extend our analysis to the case of stochastic homogenization and prove a gamma-convergence result for stationary random integrands.

## [05141] Anomalous diffusion of a passive tracer advected by the curl of the GFF in 2D

**Format :** Talk at Waseda University

**Author(s) :** Peter Morfe (Max Planck Institute, Leipzig)Georgiana Chatzigeorgiou (Max Planck Institute, Leipzig)Lihan Wang (Max Planck Institute, Leipzig)Felix Otto (Max Planck Institute, Leipzig)

**Abstract :** I will discuss the long-time asymptotics of the displacement of a passive tracer in a (time-independent) turbulent flow, where the velocity field equals the curl of the GFF, in two dimensions. Physicists long ago predicted that the mean-squared displacement scales like time with a logarithmic correction. In our contribution, we prove that this is indeed the case via a novel iterative argument that exploits fundamental ideas from the theory of stochastic homogenization.

## [04734] Variance reduction methods in random homogenization by using surrogate models

**Format :** Online Talk on Zoom

**Author(s) :** Frederic Legoll (Ecole des Ponts ParisTech and Inria)Sebastien Brisard (Ecole des Ponts ParisTech)Michael Bertin (Ecole des Ponts ParisTech and Inria)

**Abstract :** We consider the homogenization of elliptic PDEs with random coefficients. The associated corrector problem is set on the entire space, and is thus practically intractable. A standard approximation consists in restricting this problem to a large but bounded domain. The obtained effective coefficients are random. It is thus natural to consider several realizations.

To improve the accuracy on the expectation of the effective coefficients, we introduce a variance reduction approach based on a surrogate model.

## [00552] Homogenization theory and applications

**Session Time & Room :** 5D (Aug.25, 15:30-17:10) @G501

**Type :** Proposal of Minisymposium

**Abstract :** The aim of this mini-symposium is to overview contemporary theory and applications on homogenization by specialists from various areas.

Short time behavior of particles in inhomogeneous media may depend on the location of particles, whereas their long time behavior often tends to be homogeneous due to the averaging effects. Such an averaging process is called homogenization.

Homogenization has been a very active research area in mathematics and applied mathematics for a long time. We invite specialists from several fields, including PDE, probability, analysis and applied mathematics. We exchange ideas and discuss various aspects on homogenization.

**Organizer(s) :** Takashi Kumagai

**Classification :** 35B27, 74Q05, 60K37, 35J15

**Minisymposium Program :**

00552 (1/1) : 5D @G501 [Chair: Takashi Kumagai]

## [01750] On the rate of convergence in homogenization of time fractional Hamilton-Jacobi equations

**Format :** Talk at Waseda University

**Author(s) :** Hiroyoshi Mitake (University of Tokyo)

**Abstract :** In this talk, we consider periodic homogenization for time fractional Hamilton-Jacobi equations. By using the perturbed test function method, we establish the convergence, and give estimates on the rate of convergence. A main difficulty is the incompatibility between the function used in the doubling variable method, and the non-locality of the Caputo derivative. Our approach is to provide a lemma to prove the rate of convergence without the doubling variable method with respect to the time variable, which is a key ingredient. This is a joint work with Shioichi Sato (U. Tokyo).

## [01811] Discrete approximation of higher degree Laplacians

**Format :** Talk at Waseda University

**Author(s) :** Jun Masamune (Tohoku University) Hiroki Fukagawa (DeepFlow Inc)

**Abstract :** In this talk, we review some basic ideas in the theory of homogenization and discuss recent progress in the theory and applications of discrete approximation of equations involving, possibly higher degree, Laplacian. The talk is based on a collaborative effort with Hiroki Fukagawa from DeepFlow Inc.

## [03559] Homogenization of the rate-independent evolution of a random heterogeneous, elasto-plastic spring network

**Format :** Talk at Waseda University

**Author(s) :** Stefan Neukamm (TU Dresden)

**Abstract :** We consider a periodic network composed of elasto-plastic spring with stationary and ergodic coefficients, described as a evolutionary rate independent system (ERIS) and derive a homogenized, continuum model as evolutionary Gamma-limit. The limit can be described as a generalized Prandtl-Ishlinskii hysteresis model and we analyse a corresponding RVE approximation.

## [00554] Pattern dynamics appearing in mathematical biology

**Session Time & Room :** 4E (Aug.24, 17:40-19:20) @G406

**Type :** Proposal of Minisymposium

**Abstract :** Biological phenomenon have promoted the mathematical studies of pattern dynamics, such as Turing's pattern formation and traveling wave. We will introduce some of the recent progress around this topic which offer new viewpoints. We hope this is going to be the starting point to discuss the future perspective.

**Organizer(s) :** Chiun-Chuan Chen, Yoichiro Mori, Hirokazu Ninomiya, Toshiyuki Ogawa

**Classification :** 35B32, 35B36, 35K55, 35K57

**Minisymposium Program :**

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00554 (1/1) : 4E @G406 [Chair: Toshiyuki Ogawa, Hirokazu Ninomiya]

## [01234] Turing's instability by equal diffusion

**Format :** Talk at Waseda University

**Author(s) :** Hirokazu Ninomiya (Meiji University)

**Abstract :** In 1952, Turing proposed the mechanism of pattern formation in which a stable equilibrium of some kinetic system is destabilized by diffusion. In the case of two-component reaction-diffusion systems, however, the diffusion coefficients should be different. This talk presents an example of a two-component kinetic system with a asymptotically stable equilibrium, while the corresponding reaction-diffusion system has a family of unstable stationary solutions that is arbitrarily close to the homogeneous stationary solution.

## [01275] Reaction-diffusion fronts in funnel-shaped domains

**Format :** Talk at Waseda University

**Author(s) :** Mingmin Zhang (Universite Toulouse III - Paul Sabatier)

**Abstract :** We study large-time dynamics of entire solutions to bistable equations in funnel-shaped domains emanating from a planar front in the straight part and moving into the conical part. We prove a dichotomy between blocking and spreading, and show that any spreading solution is a transition front whose level sets have roughly expanding spherical shapes at large times. We provide sufficient conditions on geometry of the domains, under which the solution is blocked or spreads completely.

## [01442] Traveling wave solution in a macroscopic traffic model

**Format :** Talk at Waseda University

**Author(s) :** Kota Ikeda (Meiji University) Meiji University

**Abstract :** Various subjects in traffic dynamics have long posed a challenge. Theoretical approaches have revealed the localized and extended forms of congestion with the propagation velocity of stop-and-go waves in models. In 2001, Lee et

al. derived a macroscopic traffic model from an OV model and numerically showed that a traveling pulse appears under a relatively high density of cars. We prove the existence of such a traveling pulse rigorously via a phase plane method.

### [03160] Bistable pulsating fronts in showling oscillating environments

**Format :** Talk at Waseda University

**Author(s) :** Weiwei Ding (South China Normal University)

**Abstract :** In this talk, I will present some progress on reaction-diffusion fronts in spatially periodic bistable media. The results include: existence of pulsating fronts with large periods, existence of and an explicit formula for the limit of front speeds as the spatial period goes to infinity, convergence of pulsating front profiles to a family of front profiles associated with spatially homogeneous equations. This talk is based on joint work with Francois Hamel and Xing Liang.

## [00555] Advanced Numerical Methods for PDEs with Applications

**Session Time & Room :**

00555 (1/2) : 4C (Aug.24, 13:20-15:00) @E705

00555 (2/2) : 4D (Aug.24, 15:30-17:10) @E705

**Type :** Proposal of Minisymposium

**Abstract :** Numerical modeling and algorithms are fundamental building blocks in computational science and engineering that provide accurate and efficient solution methods to the model equations. As applications become more complex, the model equations become more difficult and sophisticated. New and efficient numerical techniques are hence needed to solving the physical equations. The goal of this mini-symposium is to present the recent developments of computational methods for applications. The topics include numerical methods for PDEs, fast solvers, adaptive methods, and software developments. The mini-symposium will emphasize both the design and analysis of numerical algorithms as well as applications in science and engineering.

**Organizer(s) :** Justin Wan, Lilia Krivodonova

**Classification :** 65Mxx, 65Nxx, 65-04, 65Jxx, Numerical PDEs, domain decomposition method, multigrid method, computational fluid dynamics, numerical software library

**Minisymposium Program :**

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00555 (1/2) : 4C @E705 [Chair: Lilia Krivodonova]

### [02041] Numerical Methods for PDEs and Mesh Generation

**Format :** Talk at Waseda University

**Author(s) :** Justin Wan (University of Waterloo)Connor Tannahill (University of Waterloo)

**Abstract :** We will start with an overview of the mini-symposium. Then, in this talk, we will present a novel optimization-based approach for variational mesh adaptation based on MMPDE methods, combined with recent techniques for solving large-scale nonlinear constraint problems in parallel. The resulting method resembles meshing algorithms based on the spring analogy while producing high-quality adaptive meshes. We demonstrate the advantages of our method over standard MMPDE methods for generating two and three-dimensional meshes in parallel.

### [01595] PDAEs redux

**Format :** Talk at Waseda University

**Author(s) :** Uri Michael Ascher (University of BC)

**Abstract :** We re-examine computational principles for solving constrained PDEs in large applications.

One involves simulation of friction and contact effects in deformable object motion arising in graphics and robotics.

The need to flexibly engage such constraints in differentiable models prompts introducing penalty methods, despite some additional complexity and minor potential instability.

The other project investigates, in the context of neural ODEs,

different stabilization methods for differential equations with invariants arising from elimination of algebraic constraints.

## [02132] Optimized Schwarz domain decomposition for surface intrinsic positive Helmholtz equations

**Format :** Talk at Waseda University

**Author(s) :** Alireza Yazdani (Simon Fraser University)Ronald Haynes (Memorial University of Newfoundland)Steven Ruuth (Simon Fraser University)

**Abstract :** We consider the convergence of optimized Schwarz iterations for the surface intrinsic positive Helmholtz equation  $(c - \Delta_S)u = f$ ,  $c > 0$ , for smooth, simple closed 1-manifolds where periodicity is inherent in the geometry. We prove convergence results for the unequal-sized subdomain case with an arbitrary number of subdomains, and find an explicit formula for the optimal Robin parameter. Connections to a particular discretization, the closest point method, are provided as are numerical experiments verifying our results.

## [02719] DD approaches for surface PDEs solved by the closest point method

**Format :** Online Talk on Zoom

**Author(s) :** Ronald Haynes (Memorial University of Newfoundland and Labrador)

**Abstract :** The solution of surface intrinsic PDEs using the closest point method will be proposed. For efficiency we have designed and analyzed domain decomposition solvers and preconditioners to solve the resulting discrete system of equations. Numerical results for model test examples will be presented.

00555 (2/2) : 4D @E705 [Chair: Justin Wan]

## [02811] TVD property of second order method for two-dimensional scalar conservation laws

**Format :** Talk at Waseda University

**Author(s) :** Lilia Krivodonova (University of Waterloo)Alexey Smirnov (University of Waterloo)

**Abstract :** The total variation diminishing (TVD) property plays a crucial role in ensuring the stability and convergence of numerical solutions for one-dimensional scalar conservation laws. It was established in 1985 that in the two-dimensional space, a TVD method can be at most first order accurate. We consider a new definition of TV and propose a condition on scheme coefficients for a second-order method to be TVD for nonlinear scalar conservation laws.

## [02206] Using Adaptive Time-Steppers to Explore Stability Domains

**Format :** Talk at Waseda University

**Author(s) :** Mary Pugh (University of Toronto)

**Abstract :** Stability domains for ODE time-steppers are well-understood when the linearized system is diagonalizable. I'll discuss an implicit-explicit time-stepper for which the linearized system isn't diagonalizable. An adaptive time-stepper can be used to explore the stability domain. I'll present a system whose stability domain has a discontinuous boundary; a small change in a parameter can cause a jump in the time-step-size stability threshold. This is joint work with my former PhD student, Dave Yan.

## [02320] Extended Statistical Modelling and Advanced Computational Approaches for Disperse Multiphase Flows

**Format :** Talk at Waseda University

**Author(s) :** Lucian Ivan (Canadian Nuclear Laboratories)Benoit Allard (University of Ottawa)Francois Forgues (Canadian Nuclear Laboratories)James McDonald (University of Ottawa)

**Abstract :** This talk presents an Eulerian-based polydisperse Gaussian-moment model (PGM) family for the description of particle-laden multiphase flows. The modelling approach leads to a set of first-order, robustly-hyperbolic balance laws that provide a direct treatment for local higher-order statistics, such as covariances between particle distinguishable properties (e.g., diameter, temperature, etc.) and particle velocity. A massively parallel discontinuous-Galerkin-Hancock framework is employed to efficiently obtain computational PGM-solutions for a range of flows, including bio-aerosol dispersion and fuel sprays.

## [02260] tost.II: A temporal operator splitting template library for deal.II

**Format :** Talk at Waseda University

**Author(s) :** Raymond Spiteri (University of Saskatchewan)Kevin Green (University of Saskatchewan)

**Abstract :** Operator splitting is a popular and often necessary means for solving PDEs. Software that implements operator splitting, however, generally

only allows specific splitting methods, with only specific sub-integrators, and only for specific problems. In this talk, I describe the `tost.II` temporal operator splitting library built on the `deal.II` finite-element library. `tost.II` enables easy experimentation with splittings for an arbitrary number of operators and with arbitrary order of convergence, including methods with negative or complex coefficients.

## [00558] Bifurcations, periodicity and stability in fluid-structure interactions

### **Session Time & Room :**

00558 (1/3) : 1C (Aug.21, 13:20-15:00) @E820

00558 (2/3) : 1D (Aug.21, 15:30-17:10) @E820

00558 (3/3) : 1E (Aug.21, 17:40-19:20) @E820

### **Type :** Proposal of Minisymposium

**Abstract :** This minisymposium connects rigorous mathematical theory with empirically observed time-periodic phenomena arising in fluid-structure interactions. Scenarios of interest include: aeroelastic resonances and flutter instabilities, e.g., bridge deck and flight-structure instabilities, and nonlinear phenomena such as von Karman vortex sheets, and the various approaches which have been developed such as spectral analyses and theories of weak solutions. Theoretical advances are complemented by progress in numerical simulation. We facilitate the connections between experts of various mathematical backgrounds for the development of new strategies exploiting the interplay between different approaches. Lastly, we wish to emphasize open problems in this challenging and exciting area.

**Organizer(s) :** Boris Muha, Sebastian Schwarzacher, Justin Webster

**Classification :** 74F10, 35Q35, 70K20, 35B40, 65Mxx

### **Minisymposium Program :**

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00558 (1/3) : 1C @E820 [Chair: Sebastian Schwarzacher]

## [04678] Weak solutions in fluid-structure interactions: Cauchy and periodic problems

### **Format :** Talk at Waseda University

**Author(s) :** Boris Muha (University of Zagreb)Sebastian Schwarzacher (Charles University and Uppsala University)Justin Thomas Webster (University of Maryland, Baltimore County)

**Abstract :** In this talk, we will provide an overview of the latest developments in the theory of weak solutions to fluid-structure interaction problems. We will specifically explore the difficulties and distinctions that arise when moving from the Cauchy problem to that of obtaining periodic solutions. We will examine a simple heat-wave system, which serves as a representative example for a fluid-structure interactions; for this system, we present some new existence results for periodic solutions.

## [02192] Modelling and analysis of solids floating in a viscous fluid

### **Format :** Talk at Waseda University

**Author(s) :** Marius Tucsnak (University of Bordeaux)

**Abstract :** We describe some recent advances on the mathematical modelling of the interaction of water waves with floating objects. The main applications we have in mind are point absorber type devices for producing marine energy and floating platforms used to support wind turbines. The mathematical challenge here is the existence of two free boundaries: the free surface of the fluid and the solid-fluid interface. The presentation is essentially devoted to wellposedness and large time behavior issues.

## [02207] Time-periodic solutions to an interaction problem between a compressible fluid and a viscoelastic structure

**Format :** Talk at Waseda University

**Author(s) :** Srđan Trifunović (Faculty of Sciences, University of Novi Sad) Šárka Nečasová (Institute of Mathematics AS CR) Ondřej Kreml (Institute of Mathematics AS CR) Václav Mácha (Institute of Mathematics AS CR)

**Abstract :** In this lecture, I will talk about the problem of interaction between a compressible fluid and a viscoelastic beam under the influence of time-periodic external forces in 2D. For this problem, at least one weak solution is constructed which is periodic in time and preserves the mass which is a given constant. The approximate solution is obtained via a decoupling scheme in finite bases for time and space.

## [02722] Artificial boundary conditions for time-periodic flow past a body

**Format :** Talk at Waseda University

**Author(s) :** Thomas Eiter (Weierstrass Institute for Applied Analysis and Stochastics)

**Abstract :** Consider the time-periodic viscous flow past an obstacle. Numerical implementations require to reduce the problem to a bounded domain by introducing an artificial boundary. In this talk, we study a choice of associated boundary conditions such that this perturbed problem suitably approximates the original one. These boundary conditions reflect the asymptotic behavior of the flow, which is studied in terms of new representation formulas relying on time-periodic fundamental solutions to the linearized Navier-Stokes equations.

00558 (2/3) : 1D @E820 [Chair: Justin Webster]

## [04833] On the motion of several small rigid bodies in a viscous incompressible fluid

**Format :** Talk at Waseda University

**Author(s) :** Eduard Feireisl (Czech Academy of Sciences)

**Abstract :** We consider the motion of  $N$  rigid bodies immersed in a viscous incompressible fluid contained in a domain in the Euclidean space  $R^d$ ,  $d = 2; 3$ . We show the fluid flow is not influenced by the presence of the bodies in the asymptotic limit as when the radius of the bodies tends to zero sufficiently fast. The result depends solely on the geometry of the bodies and is independent of their mass densities. Collisions are allowed and the initial data are arbitrary with finite energy.

## [05105] On the motion of a fluid-filled elastic solid

**Format :** Talk at Waseda University

**Author(s) :** Giusy Mazzone (Queen's University)

**Abstract :** Consider the physical system constituted by an elastic solid with an interior cavity entirely filled by a viscous incompressible fluid. The motion of the coupled system is governed by the Navier equations of linear elasticity for the solid, and the Navier-Stokes equations for the fluid. Continuity of stresses and velocities are imposed at the fluid-solid interface, while a zero-traction condition is imposed at the other free boundary of the solid. I will present some results on the existence of strong solutions to the governing equations and discuss their stability properties.

## [05124] Gevrey regularity of a certain fluid-structure PDE interaction

**Format :** Talk at Waseda University

**Author(s) :** George Avalos (University of Nebraska-Lincoln)

**Abstract :** In this talk, we present recent results concerning the qualitative behavior of a coupled partial differential equation (PDE) system which describes a certain fluid-structure interaction (FSI), as it occurs in nature. With respect to the associated strongly continuous contraction semigroup for this model, we present our recent results of Gevrey regularity.

## [05184] Numerical benchmarking of FSI - efficient discretization and numerical solution

**Format :** Online Talk on Zoom

**Author(s) :** Jaroslav Hron (Charles University, Prague)

**Abstract :** The lecture will give an overview of the problem of fluid-structure interaction motivated by blood flow in deformable vessels. Possible discretizations by the finite element method and different coupling strategies will be discussed with a focus on the efficient numerical solution of the monolithic problem. We will discuss some simple

benchmark type problems of fluid structure interaction based on finding a suitable simple arrangement with self-induced oscillations.

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00558 (3/3) : 1E @E820

## [00559] DNB Theory and its Applications

**Session Time & Room :**

00559 (1/3) : 1C (Aug.21, 13:20-15:00) @G302

00559 (2/3) : 1D (Aug.21, 15:30-17:10) @G302

00559 (3/3) : 1E (Aug.21, 17:40-19:20) @G302

**Type :** Proposal of Minisymposium

**Abstract :** The concept of dynamical network biomarker (DNB) was proposed to provide early-warning signals of diseases on the basis of co-dimension 1 local bifurcation in 2012, and then is widely used in various topics and fields of biology and medicine, e.g. dynamical analyses of biological processes in biology and disease prediction/early-diagnoses in medicine. The DNB is a novel type of biomarkers to identify the critical state during disease progression, which quantifies biological systems from a dynamical and network viewpoint, thus providing reliable information on early-warning signals before onset of complex diseases. Many DNB methods as well as applications have been developed. The DNB theory with big biological data is expected to lead to ultra-early precision and preventive medicine. This symposium addresses but not limited to the recent development of theory, methodology and application of DNB in a variety of scientific areas.

**Organizer(s) :** Kazuyuki Aihara, Luonan Chen

**Classification :** 03Cxx, 37-xx, 92-xx

**Minisymposium Program :**

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00559 (1/3) : 1C @G302

### [05641] DNB-based intervention for ultra-early treatment

**Format :** Talk at Waseda University

**Author(s) :** Jun-ichi Imura (Tokyo Institute of Technology)

**Abstract :** The process leading to the onset of disease may be understood as a rapid transition in the complex interactions between genes. This talk proposes a DNB-based intervention approach for preventive treatment just before such transitions, i.e., in the pre-disease state, by combining DNB theory with control theory to build a theory that estimates which nodes of the relevant gene expression network should be intervened and how they should be intervened.

### [05637] Alerting for the critical transition of complex systems

**Format :** Talk at Waseda University

**Author(s) :** Rui Liu (South China University of Technology)

**Abstract :** It is a challenging task to accurately predict the future critical state of a short-term time-series. The major difficulty to solve such a task is the lack of the information, which typically results in the failure of most existing approaches due to the overfitting problem of the small sample size. To address this issue, we proposed a computing framework: auto-reservoir neural network, to efficiently and accurately make the multi-step-ahead prediction based on a short-term high-dimensional time-series. Different from traditional reservoir computing whose reservoir is an external dynamical system irrelevant to the target system, ARNN directly transforms the observed high-dimensional dynamics as its reservoir, which maps the high-dimensional/spatial data to the future temporal values of a target variable based on a spatiotemporal information (STI) transformation. Combining with the dynamic network biomarker (DNB), it is possible to detect the early-warning signal of critical transitions of real-world complex systems.

### [05638] The algorithm and application of landscape-DNB in complex disease of single sample

**Format :** Talk at Waseda University

**Author(s) :** Xiaoping Liu (Hangzhou Institute for Advanced Study)

**Abstract :** A new model-free method has been developed and termed the landscape dynamic network biomarker (l-DNB) methodology. The method is based on bifurcation theory, which can identify tipping points prior to serious disease deterioration using only single-sample omics data. Here, we show that l-DNB provides early-warning signals of disease deterioration on a single-sample basis and also detects critical genes or network biomarkers (i.e. DNB members) that

promote the transition from normal to disease states. As a case study, l-DNB was used to predict severe influenza symptoms prior to the actual symptomatic appearance in influenza virus infections. The l-DNB approach was then also applied to three tumor disease datasets from the TCGA and was used to detect critical stages prior to tumor deterioration using an individual DNB for each patient. The individual DNBs were further used as individual biomarkers in the analysis of physiological data, which led to the identification of two biomarker types that were surprisingly effective in predicting the prognosis of tumors. The biomarkers can be considered as common biomarkers for cancer, wherein one indicates a poor prognosis and the other indicates a good prognosis.

## [05640] DNB based network fluctuation and application to biology and medicine

**Format :** Talk at Waseda University

**Author(s) :** Luonan Chen (Chinese Academy of Sciences)

**Abstract :** I will talk about the recent progress on the DNB methods as well as the applications to biology and medicine. By exploring the original DNB concept, i.e. critical collective fluctuation (CCF) of the observed variables, we developed a network flow entropy, which can quantify the CCF so as to detect the tipping point before the critical transition from one stable equilibrium to another. The applications include the tipping points of various diseases.

00559 (2/3) : 1D @G302

## [05343] Change-point detection in temporal complex systems

**Format :** Talk at Waseda University

**Author(s) :** Huanfei Ma (Soochow University)

**Abstract :** We develop a model-free approach, named temporal change-point detection (TCD), and integrate both dynamical and statistical methods to achieve accurate detection of the time instant at which a system changes its internal structures. The proposed approach is able not only to detect the separate change points of the concerned systems without knowing, a priori, any information of the equations of the systems, but also to harvest all the change points emergent in a relatively high-frequency manner.

## [05648] Early warning signals for multistage transitions in tipping dynamics on networks

**Format :** Talk at Waseda University

**Author(s) :** Neil G. MacLaren (State University of New York at Buffalo)Prosenjit Kundu (State University of New York at Buffalo)Naoki Masuda (State University of New York at Buffalo)

**Abstract :** Complex dynamical systems for which we want to anticipate sudden regime shifts often form a heterogeneous network. We propose methods to select sentinel nodes in a given network to construct informative early warning signals given that the network may be heterogeneous and show multistage transitions. We show that small subsets of nodes can anticipate transitions as well as or even better than using all the nodes under the proposed node selection method. Informative sentinel nodes depend on the direction of regime shifts, which we also highlight in the talk.

## [03348] Modelling single cell multi-omics data

**Format :** Talk at Waseda University

**Author(s) :** Yong Wang (Academy of Mathematics and Systems Science, Chinese Academy of Sciences)

**Abstract :** In this talk I will introduce combinatorial regulon (cRegulon) to model the combinations among TFs, which can better characterize cell types and serves as the driving forces for cell state transitions. By leveraging rapidly accumulated single multi-omics data, we develop an optimization model to systematically infer cRegulons (i.e., the representative TF modules, their associated regulatory elements and target genes formed regulatory network).

00559 (3/3) : 1E @G302

## [00563] PDE's on Mathematical Physics and Biology

**Session Time & Room :**

00563 (1/2) : 3D (Aug.23, 15:30-17:10) @G709

00563 (2/2) : 3E (Aug,23, 17:40-19:20) @G709

**Type :** Proposal of Minisymposium

**Abstract :** This minisymposium will be focused on different models concerning mathematical biology and mathematical physics, both from an analytical and applied point of view.

In the first part, we will give an overview on different problems in population dynamics, such as invasion, spreading of populations and living in regions or in graphs.

The second part will deal with problems involving the Schrödinger operator, coming from mathematical Physics. Precisely, it will be discussed results such as existence of ground state solutions and stability of solutions.

**Organizer(s) :** Pablo Álvarez-Caudeville, Cristina Brändle, Eduardo Colorado, Tatsuya Watanabe

**Classification :** 35Q55, 35Q92, 35J60

**Minisymposium Program :**

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00563 (1/2) : 3D @G709 [Chair: Tatsuya Watanabe]

## [04143] The effect of diffusion on principal eigenvalues for Hamilton-Jacobi equations

**Format :** Talk at Waseda University

**Author(s) :** Cristina Brändle (U. Carlos III Madrid)

**Abstract :** We deal with the ergodic problem of viscous Hamilton–Jacobi equations with superlinear Hamiltonian, inward-pointing

drift and a positive potential function that vanishes at infinity. We characterize the generalized principal eigenvalue with respect to diffusion and also specify the necessary and sufficient condition so that the spectral function contains a plateau.

## [03901] Population models with an interface region inside the domain

**Format :** Talk at Waseda University

**Author(s) :** Pablo Alvarez-Caudeville (Universidad Carlos III de Madrid) Pablo Alvarez Caudeville (Universidad Carlos III de Madrid)

**Abstract :** We will discuss several models that might be regarded as migration models of populations moving from one part of a domain to the other and becoming part of the population living on the other side. Different situations assuming symmetry of movement between both sides of the domain, following a logistic model in their own environment and assuming spatial heterogeneities, are going to be discussed. Through such a common boundary both populations are coupled, acting as a permeable membrane on which their flow moves in and out.

We will describe the precise interplay between the stationary solutions with respect to the parameters involved in the problem, in particular the growth rate of the populations and the coupling parameter involved on the boundary where the interchange of flux is taking place.

## [04005] A bifurcation result for a fractional semilinear Neumann problem

**Format :** Talk at Waseda University

**Author(s) :** Luca Vilasi (University of Messina)

**Abstract :** We will examine a parameterized elliptic problem governed by the Neumann fractional Laplacian on a bounded domain of  $\mathbb{R}^N$ ,  $N \geq 1$ , with a general nonlinearity. This problem arises, in particular, when looking for steady state solutions to Keller-Segel systems in which the diffusion of the chemical is non-local. By variational arguments we will show the existence of non-trivial solutions, local minima of the corresponding energy functional, that branch off the null one for small values of the parameter. We will also derive some regularity results, as well as other qualitative properties of the solutions.

## [04254] Systems of coupled nonlinear Schrödinger equations

**Format :** Talk at Waseda University

**Author(s) :** Eduardo Colorado (Universidad Carlos III de Madrid)

**Abstract :** Along the talk we will see some results about existence of solutions to general coupled systems of nonlinear Schrödinger (NLS) equations (and systems of coupled NLS-nonlinear Korteweg-de Vries equations).

To do so, we will use variational techniques once one pass to the elliptic system obtained by looking for standing solitary wave solutions (or standing-travelling wave solutions) for the NLS coupled system (or the NLS-NKdV coupled system).

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00563 (2/2) : 3E @G709 [Chair: Pablo Álvarez-Caudeville]

## [03153] Stable standing waves for a Schrödinger system with nonlinear chi^3 response

**Format :** Talk at Waseda University

**Author(s) :** Tatsuya Watanabe (Kyoto Sangyo University)

**Abstract :** In this talk, we consider standing wave solutions for a certain nonlinear Schrodinger system which appears in nonlinear optics. This two-component system contains a cubic nonlinear term which is called  $\chi^3$ -interaction, and has a strong coupling on one side only.

Oliveira-Pastor (2021) showed the existence of ground state solutions for the corresponding stationary problems, and investigated their stability and instability. In our study, by considering the solvability of a constraint minimization problem, we show the existence of stable standing wave solutions. We also investigate the correspondence between minimizers and ground state solutions.

This work is based on joint research with Mathieu Colin (University of Bordeaux).

## [03664] Critical nonlocal problems driven by the fractional Laplacian

**Format :** Online Talk on Zoom

**Author(s) :** Raffaella Servadei (Università degli Studi di Urbino Carlo Bo)

**Abstract :** Critical problems are particularly relevant for their relations with many applications where a lack of compactness occurs.

The fractional Laplacian operator appears in concrete applications in many different fields. This is one of the reason why, recently, nonlocal fractional problems are widely studied in the literature.

Aim of this talk is to discuss some recent results about existence and multiplicity of solutions for fractional nonlocal equations with critical growth assumptions on the nonlinear term.

## [04405] Variational and topological methods on non-compact Randers spaces

**Format :** Online Talk on Zoom

**Author(s) :** Giovanni Molica Bisci (University of Urbino Carlo Bo)

**Abstract :** Motivated by a wide interest in the literature, the leading purpose of this talk is to present some recent abstract results on non-compact Randers spaces and their applications to quasilinear elliptic equations. The main approach is based on novel abstract Sobolev embedding results as well as on some variational and topological methods.

## [00570] Title: Machine Learning and Statistical Approaches for PDE Based Inverse Problems in Imaging

**Session Time & Room :**

00570 (1/2) : 4C (Aug.24, 13:20-15:00) @E503

00570 (2/2) : 4D (Aug.24, 15:30-17:10) @E503

**Type :** Proposal of Minisymposium

**Abstract :** In recent years, there is tremendous growth in machine learning and statistical approaches to solve inverse problems involving PDEs. This mini symposium will explore ideas both theoretical and computational to advance understanding of the convergence, consistency, and numerical algorithms to solve PDE based inverse problems. We will focus on inverse problems with applications to imaging including Electrical Impedance Tomography, Diffuse Optical Tomography. The mini symposium is expected to bring experts from theory, computation, and practice to bridge the gap between these areas.

**Organizer(s) :** Department of Mathematics and Statistics, University of North Carolina at Charlotte, USA

**Classification :** 62G20, 35J15, 62F15

**Minisymposium Program :**

00570 (1/2) : 4C @E503 [Chair: Taufiquar Khan]

## [04498] Train Like a (Var)Pro: Efficient Training of DNNs

**Format :** Talk at Waseda University

**Author(s) :** Elizabeth Newman (Emory University)Lars Ruthotto (Emory University)Bart van Bloemen Waanders (Sandia National Laboratories)Joseph Hart (Sandia National Laboratories)

**Abstract :** Deep neural networks (DNNs) have excelled as high-dimensional function approximators and are trained by solving a challenging stochastic optimization problem. In this talk, we will make DNN training easier by exploiting separability of common architectures; i.e., linear in the final weights. We will leverage this linearity by eliminating the weights through variable projection. We will demonstrate the efficacy of this approach through numerical examples and will conclude with a discussion of extensions and new applications.

## [05369] Machine Learning for Inverse Problems in Electrical Impedance Tomography

**Format :** Talk at Waseda University

**Author(s) :** Hyeuknam Kwon (Yonsei University, Mirae campus)

**Abstract :** This paper discusses the application of machine learning techniques to solve inverse problems in electric impedance tomography (EIT). EIT is a non-invasive medical imaging technique used to reconstruct the distribution of conductivity within the human body using electrical measurements of surfaces. However, the inverse problem in EIT image reconstruction and its application suffers from various difficulties. The author provides these problems and machine learning techniques to solve them.

00570 (2/2) : 4D @E503 [Chair: Taufiquar Khan]

## [04986] Data-Driven Design of Thin-Film Optical Systems using Deep Active Learning

**Format :** Talk at Waseda University

**Author(s) :** Youngjoon Hong (Sungkyunkwan University)

**Abstract :** A deep learning aided optimization algorithm for the design of flat thin-film multilayer optical systems is developed. We introduce a deep generative neural network, based on a variational autoencoder, to perform the optimization of photonic devices. This algorithm allows one to find a near-optimal solution to the inverse design problem of creating an anti-reflective grating, a fundamental problem in material science. As a proof of concept, we demonstrate the method's capabilities for designing an anti-reflective flat thin-film stack consisting of multiple material types. We designed and constructed a dielectric stack on silicon that exhibits an average reflection, which is lower than other recently published experiments in the engineering and physics literature. In addition to its superior performance, the computational cost of our algorithm based on the deep generative model is much lower than traditional nonlinear optimization algorithms. These results demonstrate that advanced concepts in deep learning can drive the capabilities of inverse design algorithms for photonics. In addition, we develop an accurate regression model using deep active learning to predict the total reflectivity for a given optical system. The surrogate model of the governing partial differential equations can then be broadly used in the design of optical systems and to rapidly evaluate their behavior.

## [04138] Implicit Solutions of Electrical Impedance Tomography Using Deep Neural Network

**Format :** Talk at Waseda University

**Author(s) :** Taufiquar Khan (UNC Charlotte)Thilo Strauss (Bosch)

**Abstract :** In this talk, we will discuss deep learning approach for the electrical impedance tomography (EIT). In the last several decades, researchers have made significant improvement for image reconstruction for the EIT inverse problem. However, there is still need for much improvement. In this talk, we will discuss a shape reconstruction approach using machine learning. We propose a neural network architecture where the neural network model estimates the probability for a point of whether the conductivity belongs to the background region or to the non-homogeneous region. We present our numerical results to show the performance of the architecture and compare the proposed method with other known algorithms.

# [00571] Mathematics in biological pattern formation: modeling, analysis, and applications

**Session Time & Room :** 3D (Aug.23, 15:30-17:10) @G501

**Type :** Proposal of Minisymposium

**Abstract :** This mini-symposium will focus on recent advances in mathematical modeling and analysis of pattern formation problems related to biology. Mainly, we will discuss how to explain pattern formation through the analysis of the evolution equations such as ODE and PDE, which are modeled to fit the context of the biological phenomena. In this mini-symposium, we will invite researchers working on different types of model equations, such as particle systems, reaction-diffusion systems, and Fokker-Planck equations, to introduce a variety of approaches to pattern formation problems in biology.

**Organizer(s) :** Shin-Ichiro Ei, Hiroshi Ishii

**Classification :** 35B36, 92B05, 92C15, Pattern formation problem in biology

**Minisymposium Program :**

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00571 (1/1) : 3D @G501 [Chair: Shin-Ichiro Ei, Hiroshi Ishii]

## [04548] Patterning conditions in bilayer reaction-cross-diffusion systems

**Format :** Talk at Waseda University

**Author(s) :** Antoine Diez (Kyoto University Institute for the Avanced Study of Human Biology (ASHBi))Andrew L. Krause (Durham University)Philip K. Maini (University of Oxford)Eamonn A. Gaffney (University of Oxford)Sungrim Seirin-Lee (Kyoto University)

**Abstract :** Various biological systems such as the skin can be modelled by reaction-cross-diffusion networks in a so-called bilayer geometry where two independent reaction-cross-diffusion systems are coupled by a linear transport law. This work considers an arbitrary number of reacting species and gives quantitative theoretical asymptotic conditions, supported by numerical simulations, under which the coupling itself triggers patterning or stabilizes a homogeneous equilibrium.

## [04979] Multilevel mathematical modeling methods for morphogenesis of bacterial cell populations

**Format :** Talk at Waseda University

**Author(s) :** Sohei Tasaki (Hokkaido University)Madoka Nakayama (Hokkaido University)Masaharu Nagayama (Hokkaido University)Izumi Takagi (Tohoku University)

**Abstract :** Bacterial cell populations exhibit diverse growth morphologies and collectively form a robust system that can withstand environmental fluctuations. The diversity of macroscopic spatiotemporal patterns and flexible environmental responses in morphogenesis are supported by a variety of cellular states. Therefore, to understand the morphogenesis of bacterial populations, it is necessary to construct and analyze multilevel mathematical models that connect the cellular and tissue levels. Here we propose two multilevel modeling methods.

## [04657] A continuous model for bacteria growth with short range interactions, growth and interaction: derivation and analysis of pattern formation

**Format :** Talk at Waseda University

**Author(s) :** Sophie Hecht (CNRS, LJLL, Sorbonne Université)

**Abstract :** We study a mathematical model to describe the spatial evolution of micro-colony growth with bacteria of variable size. This PDE model describes the dynamics of the density of bacteria due to short-range interaction, growth, and division. We first derive the model from a many particles system by performing a large number limit followed by a localization limit. The difficulty in these limits resides in the lack of compactness according to the size variable. We then investigate the process of pattern formation in a two-dimensional domain. We analyse how the cross-diffusion inherent to the model linked to the size variable can impact the formation of spatial patterns such as size sorting.

## [03139] Approximation for nonlocal Fokker-Planck equations by a Keller-Segel system

**Format :** Talk at Waseda University

**Author(s) :** Yoshitaro Tanaka (Future University Hakodate) Hideki Murakawa (Ryukoku University)

**Abstract :** To describe biological phenomena such as cell migration and cell adhesion many models with advective nonlocal interaction have been proposed. As an attempt to construct an analysis method for these equations, we approximate the nonlocal Fokker-Planck equation by the combination of a Keller-Segel system. We show that the solution of the nonlocal Fokker-Planck equation with any even continuous integral kernel can be approximated as a singular limit of the Keller-Segel system by controlling parameters.

## [00573] Emerging Methods for Shape- and Topology Optimization

**Session Time & Room :**

00573 (1/2) : 4D (Aug.24, 15:30-17:10) @E605

00573 (2/2) : 4E (Aug.24, 17:40-19:20) @E605

**Type :** Proposal of Minisymposium

**Abstract :** Shape and topology optimization has seen considerable progress in multiple areas recently, in particular in regards to the understanding of non-smoothness and higher order methods. A driving problem class for these new developments have been inverse and reconstruction problems. The goal of this mini-symposium is to bridge the gap between these developments and connect new algorithmic developments with applications.

To this end, the first session focuses on the progression from non-smooth shape optimization problems over Quasi-Newton methods to  $H^1$  and  $H^2$  schemes, while the second part focuses on novel applications and emerging new areas of shape and topology optimization.

**Organizer(s) :** Stephan Schmidt, Roland Herzog

**Classification :** 65K10, 35R37, 49M15, 49M41, 35R30

**Minisymposium Program :**

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00573 (1/2) : 4D @E605

## [02707] Geometry Segmentation with Total Variation Regularization

**Author(s) :** Lukas Baumgärtner (Humboldt Universität zu Berlin) Ronny Bergmann (NTNU Trondheim) Roland Herzog (Uni Heidelberg) Manuel Weiß (Uni Heidelberg (IWR)) Stephan Schmidt (Humboldt-Universität zu Berlin)

**Abstract :** The total variation has proven as a useful regularizer for various applications in Inverse imaging and Shape optimization problems. For the task of shape segmentation, we consider two models that combine normal vector data of a discrete surface with a total variation penalty that is evaluated in the assignment space and the label space. We show how to solve the model problems using the Chambolle-Pock algorithm and ADMM.

## [03021] Topology optimisation with general dilatations via the topological state derivative

**Author(s) :** Phillip Baumann (TU Wien) Idriss Mazari-Fouquer (CEREMADE, Paris Dauphine Université, PSL) Kevin Sturm (TU Wien)

**Abstract :** In this work we introduce the topological state derivative, a novel approach to treat PDE-constrained topology optimisation problems. This notion allows to deal with point perturbations as well as more general perturbations like smooth hypersurfaces in a similar way. Furthermore, we draw a connection from the topological state derivative to the asymptotic expansion of the state equation, which is usually derived using boundary layer correctors. Finally, we present numerical results based on these ideas.

## [03573] Combining parameterized aerodynamic shape optimization with Sobolev smoothing

**Author(s)** : Nicolas R. Gauger (University of Kaiserslautern-Landau) Stephan Schmidt (Humboldt University Berlin) Thomas Dick (University of Kaiserslautern-Landau)

**Abstract** : On the one hand, Sobolev gradient smoothing can considerably improve the performance of aerodynamic shape optimization and prevent issues with regularity. On the other hand, Sobolev smoothing can also be interpreted as an approximation for the shape Hessian. This paper demonstrates, how Sobolev smoothing, interpreted as a shape Hessian approximation, offers considerable benefits, although the parameterization is smooth in itself already. Such an approach is especially beneficial in the context of simultaneous analysis and design, where we deal with inexact flow and adjoint solutions, also called One Shot optimization. Furthermore, the incorporation of the parameterization allows for direct application to engineering test cases, where shapes are always described by a CAD model. The new methodology presented in this paper is used for reference test cases from aerodynamic shape optimization and performance improvements in comparison to a classical Quasi-Newton scheme are shown.

## [03630] A combined phase field - Lipschitz method for PDE constrained shape optimization

**Author(s)** : Michael Hinze (Universität Koblenz) Philip Herbert (Heriot-Watt University) Christian Kahle (Universität Koblenz)

**Abstract** : Abstract: We present a general shape optimisation framework for PDE constrained shape optimization, which combines phase field methods and the method of mappings in the Lipschitz topology. In a first step the phase field approach determines the topology of the sought shape, and with the zero level set of the phase field simultaneously provides an approximation of the optimal shape. The latter serves as starting point for a sharp interface shape optimization method in the Lipschitz topology. To illustrate our approach we present a selection of PDE constrained shape optimisation problems and compare our findings to results from so far classical Hilbert space methods and recent p-Laplace -approximations.

00573 (2/2) : 4E @E605

## [04267] Interface Identification constrained by Local-to-Nonlocal Coupling

**Author(s)** : Matthias Schuster (Trier University) Christian Vollmann (Trier University) Volker Schulz (Trier University)

**Abstract** : Models of physical phenomena that use nonlocal operators are better suited for some applications than their classical counterparts that employ partial differential operators.

However, the numerical solution of these nonlocal problems can be quite expensive. Therefore, Local-to-Nonlocal couplings have emerged that combine partial differential operators with nonlocal operators.

In this talk, we make use of an energy-based Local-to-Nonlocal coupling that serves as a constraint for an interface identification problem.

## [04673] Total Generalized Variation for Geometric Inverse Problems

**Author(s)** : Lukas Baumgärtner (Humboldt Universität zu Berlin) Stephan Schmidt (Humboldt University Berlin) Roland Herzog (Heidelberg University) Ronny Bergmann (NTNU, Trondheim) Manuel Weiß (Uni Heidelberg (IWR)) Jose Vidal-Nunez (University of Alcalá de Henares)

**Abstract** : The total variation of the outer normal vector of a shape is discussed in the context of triangulated meshes embedded in 3D. This non-smooth regularizer requires an advanced algorithm to be used in (inverse) shape optimization problems. A split

Bregman/ADMM method is used for this purpose. There, the non-smooth objective is split into a smooth shape optimization problem and a simple non-smooth problem. The smooth shape problem is solved by a globalized Newton method. Due to the nature of the regularizer, the first and second-order shape derivatives can not be computed by algorithmic differentiation. Therefore, their analytic form is derived and some of their properties are discussed. Numerical results are presented for mesh denoising problems.

An extension, the total generalized variation of the normal, to counteract the so-called staircasing effect is presented.

## [04738] Choice of Inner Product in Shape Gradient Descent

**Author(s)** : Caitriona Jacqueline McGarry (University of Leicester) Alberto Paganini (University of Leicester)

**Abstract** : In optimisation problems with infinite dimensional control spaces, the choice of inner product on the control space affects the gradient, the direction of steepest descent wrt the induced norm.

Shape optimisation is no exception, with the control variable in an infinite dimensional function space. We will study the impact on shape optimisation of endowing this space of vector fields with alternatively an  $H^1$  or  $H^2$  inner product, especially regarding adding or removing corners of a shape.

### [04786] Image and Shape Registration via Transport Equations

**Author(s)** : Stephan Schmidt (University of Trier)Lukas Baumgärtner (Humboldt Universität zu Berlin)

**Abstract** : We consider the use of transport equations as a model for solving inverse and registration problems. Incorporating shape Hessians to facilitate higher order methods have recently made new classes of problems tractable, ranging from the formation of capillary bridges in particle flows to the detection of motion in medical scans as well as mesh registration problems. Special attention is given on how to treat hyperbolic constraints within the setting of moving shapes and images.

## [00574] Recent Progress on Stochastic Analysis, Control, and their Applications

**Session Time & Room :**

00574 (1/2) : 1D (Aug.21, 15:30-17:10) @D514

00574 (2/2) : 1E (Aug.21, 17:40-19:20) @D514

**Type** : Proposal of Minisymposium

**Abstract** : This minisymposium features new developments in stochastic analysis, control, and their applications. The invited speakers will be presenting results on impulse control with discontinuous setup costs, deep learning approach for optimal control, optimal control problem for regime-switching processes, and feedback control for switching diffusion systems based on discrete time observations in the first session. The second session will be focused on exponential stability and weak stability of stochastic functional differential equations with impulsive perturbations and a two-time-scale formulation as well as McKean-Vlasov stochastic differential equations. It is anticipated that this minisymposium will help to exchange ideas and stimulate further collaborations.

**Organizer(s)** : Chao Zhu

**Classification** : 93E20, 60H10, 34K50

**Minisymposium Program :**

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00574 (1/2) : 1D @D514 [Chair: Chao Zhu]

### [03197] Continuous-Review Inventory Systems with Discontinuous Setup Costs

**Format** : Talk at Waseda University

**Author(s)** : Dacheng Yao (Academy of Mathematics and Systems Science, Chinese Academy of Sciences)

**Abstract** : In this talk, we will discuss continuous-review inventory systems, in which the setup cost of each order is a discontinuous function of order quantity and the demand process is modeled as a Brownian motion with a positive drift. Assuming the holding and shortage cost to be a convex function of inventory level, we prove that an  $(s, S)$  policy is optimal among all admissible policies under the long-run average cost criterion. However, under the discounted cost criterion, we find that although some  $(s, S)$ -type policies are indeed optimal in some cases, any  $(s, S)$  policy cannot always be optimal for all initial inventory level  $x \in \mathbb{R}$  in the other cases.

### [04097] Deep learning methods in insurance and risk management

**Format** : Talk at Waseda University

**Author(s)** : Zhuo Jin (Macquarie University)

**Abstract** : Recently, deep learning approaches has drawn increasing attention in decision making processes. A type of Markov chain approximation-based iterative deep learning algorithm is developed to study the optimal control problems arising from the insurance industry. The optimal controls are approximated as deep neural networks. The framework of Markov chain approximation plays a key role in building the iterative equations and initialization of the algorithm. Optimal parameters of neural networks are then obtained iteratively.

## [04139] Exponential stability of stochastic functional differential equations with impulsive perturbations

**Format :** Talk at Waseda University

**Author(s) :** KY QUAN TRAN (SUNY Korea)George Yin (University of Connecticut)

**Abstract :** This work aims to investigate the moment exponential stability of stochastic functional differential equations subject to

impulsive perturbations and Markovian switching. In contrast to existing literature, we propose new criteria for moment exponential stability and a new method for computing moment Lyapunov exponents. Our analysis also shows that the Euler-Maruyama approximation method can effectively reproduce exponential stability in the mean square, provided that the step sizes are sufficiently small.

## [03618] Fully-coupled two-time-scale stochastic functional differential equations with infinite delay

**Format :** Talk at Waseda University

**Author(s) :** Fuke Wu (Huazhong University of Science and Technology)

**Abstract :** This paper examines the fully-coupled two-time-scale stochastic functional differential equations (SFDEs) with infinite delay. The system under consideration involves a slow component and a fast component. This paper aims to establish the averaging principle. To overcome the difficulty due to the infinite delay and the coupling of the segment process, some properties as the Hölder continuity and tightness on a space of continuous functions have to be investigated for the segment process.

00574 (2/2) : 1E @D514 [Chair: Fuke Wu]

## [03662] On the weak stability and stabilization of McKean-Vlasov stochastic differential equations

**Format :** Talk at Waseda University

**Author(s) :** Chao Zhu (University of Wisconsin-Milwaukee)

**Abstract :** This work focuses on weak stability and stabilization of a class of McKean-Vlasov stochastic differential equations (SDEs). First, under suitable conditions on the coefficients of the SDE, we derive explicit quantitative contraction rates for the convergence in Wasserstein distances of McKean-Vlasov SDEs using the coupling method. The contraction results are then used to prove a propagation of chaos uniformly in time, which provides quantitative bounds on convergence rate of interacting particle systems, and establishes exponential ergodicity for McKean-Vlasov SDEs. Finally we consider the question of stabilizing in the weak sense an arbitrary McKean-Vlasov SDE using suitable feedback controls with delays.

## [05067] Limit Theorems for Distribution Dependent Jump Processes with Random Switching

**Format :** Online Talk on Zoom

**Author(s) :** Fubao Xi (Beijing Institute of Technology)Chao Zhu (University of Wisconsin-Milwaukee)

**Abstract :** We consider distribution dependent jump processes with random switching, where the switching processes may have a countably infinite state space. By virtue of the martingale approach, we first establish the existence and uniqueness theorem of the underlying processes for a special Markovian switching case. Using a martingale function, we then transfer the existence and uniqueness result onto the general state-dependent switching case. Moreover, we establish two limit theorems for the processes with mean field interactions.

## [03342] From the optimal singular stochastic control to the optimal stopping for regime-switching processes

**Format :** Online Talk on Zoom

**Author(s) :** Jinghai Shao (Tianjin University)Taoran Tian (Tianjin University)

**Abstract :** This work generalizes the connection between optimal singular control and optimal stopping problem for regime-switching processes. Via optimal singular control, the optimal stopping time and the continuation region are characterized. Moreover, we prove the existence of optimal singular stochastic control for a finite horizon singular control problem with the cost function containing the terminal cost. We prove it directly by the compactification method. Such a problem was left open in Haussmann and Suo (SICON, 1995).

# [00575] Factors and Cycles

**Session Time & Room :** 5B (Aug.25, 10:40-12:20) @G302

**Type :** Proposal of Minisymposium

**Abstract :** Factors and cycles are well established subjects in the field of graph theory. They are basic and fundamental problems: for a given graph  $G$ , taking a regular graph as a spanning subgraph of  $G$ . On the other hand, factors and cycles have several applications in contexts including error correction coding theory, scheduling problems, wireless networking, and many others.

Regardless of efforts by mathematicians, there are many problems on factors and cycles which are not solved yet. This minisymposium intends to bring pioneer researchers to present their very recent discoveries on factors, cycles and related topics.

**Organizer(s) :** Shoichi Tsuchiya

**Classification :** 05C38, 05C45, 05C70

**Minisymposium Program :**

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00575 (1/1) : 5B @G302 [Chair: Shoichi Tsuchiya]

## [02338] On cycles and factors in graphs with large degree sum

**Format :** Talk at Waseda University

**Author(s) :** Takamasa Yashima (Seikei University)

**Abstract :** Numerous researchers have conducted investigations into a Hamiltonian cycle and related objects in both general graphs and bipartite graphs. In this talk, we will focus on two specific topics related to this field. The first topic concerns the problem of finding a spanning subgraph, also known as a factor, that satisfies certain degree constraints. The second topic concerns the problem of finding a Hamiltonian cycle containing a pre-specified set of independent edges, or a matching.

## [02275] Toughness and forbidden subgraphs for graphs to be hamiltonian

**Format :** Talk at Waseda University

**Author(s) :** Masahiro Sanka (Keio University)

**Abstract :** We say that a graph  $G$  is  $t$ -tough if for each vertex cut  $S \subset V(G)$ , the number of components of  $G - S$  does not exceed  $\frac{|S|}{t}$ . In 1973, Chvátal has conjectured that there exists a constant  $t_0$  such that every  $t_0$ -tough graph is hamiltonian. In this talk, we discuss some results on Chvátal's conjecture in  $R$ -free graphs for some graph  $R$ . In particular, we will present hamiltonicity of  $2K_2$ -free graphs and  $(K_2 \cup kK_1)$ -free graphs.

## [02216] Recent progress on distance matching extension in graphs on surfaces

**Format :** Talk at Waseda University

**Author(s) :** Jun Fujisawa (Keio University)

**Abstract :** A graph  $G$  is said to be distance  $d$  matchable if, for any matching  $M$  of  $G$  in which edges are pairwise at least distance  $d$  apart, there exists a perfect matching of  $G$  which contains  $M$ . If we choose a class of graphs  $A$  and an integer  $d$  appropriately, then we may observe a phenomenon that every graph in  $A$  is distance  $d$  matchable. In this talk recent results concerning this phenomenon is introduced.

## [02696] Eigenvalues and factors in regular graphs

**Format :** Talk at Waseda University

**Author(s) :** Suil Oh (SUNY Korea)

**Abstract :** In this talk, we investigate spectral conditions for an ( $r$ -regular) graph  $G$  to guarantee the existence of a certain factor.

# [00580] Mathematical Challenges in Current and Future Location Estimation Systems

**Session Time & Room :** 3E (Aug.23, 17:40-19:20) @E502

**Type :** Proposal of Minisymposium

**Abstract :** Location-estimation systems, and in particular Global Navigation Satellite Systems (e.g. GPS), are mature and ubiquitous. Many aspects of modern life are today completely dependent on these systems. However, deriving additional benefits (higher accuracy, resilience to jamming and spoofing) from existing systems and building future systems to fill application gaps require addressing challenging mathematical and computational problems. These challenges revolve around difficult nonconvex optimization problems, some with integer parameters, and some in high dimensions. Effective solutions require a combination of state-of-the-art mathematical tools with application-specific insights. The minisymposium will present both challenges and recent progress towards their solution.

**Organizer(s) :** Sivan Toledo, Xiao-Wen Chang

**Classification :** 62F10, 90C90, 62F35, 90C11, 90C22

**Minisymposium Program :**

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00580 (1/1) : 3E @E502 [Chair: Sivan Toledo]

## [01325] Local Strong Convexity of Source Localization and Error Bound for Target Tracking under Time-of-Arrival Measurements

**Format :** Talk at Waseda University

**Author(s) :** Anthony Man-Cho So (The Chinese University of Hong Kong)Yuen-Man Pun (The Australian National University)

**Abstract :** We consider a time-varying optimization approach to the problem of tracking a moving target using noisy time-of-arrival {TOA} measurements. To analyze the tracking performance of online gradient descent {OGD}, we first revisit the classic least-squares formulation of the {static} TOA-based source localization problem and elucidate its estimation and geometric properties. Then, we show that the loss function in the formulation, albeit non-convex in general, is locally strongly convex at its global minima. To the best of our knowledge, these results are new and can be of independent interest. By combining them with existing techniques from online strongly convex optimization, we then establish the first non-trivial bound on the cumulative target tracking error of OGD.

## [01604] Machine learning techniques for resolving GNSS integer ambiguities

**Format :** Talk at Waseda University

**Author(s) :** Xiao-Wen Chang (McGill University)Qincheng Lu (McGill University)

**Abstract :** A key computational component in high precision GNSS positioning is to resolve carrier phase ambiguities as integers. The optimal method is to solve an integer least squares problem. Since the integer least squares problem is NP-hard, efficiency of traditional algorithms becomes problematic when the dimension of the integer ambiguity vector becomes large. To meet the challenge, we propose some machine learning based algorithms. Numerical results will demonstrate their effectiveness and efficiency.

## [01656] Fast and almost unbiased position estimation for location service

**Format :** Talk at Waseda University

**Author(s) :** Peiliang Xu (Kyoto University)

**Abstract :** We propose a bias-corrected weighted LS method for precise location service, which consists of two basic elements: one to automatically correct the bias due to model nonlinearity and the induced biases in squared ranges/pseudoranges and the other to sequentially estimate unknown location parameters by treating equality constraints as a condition adjustment. The method is applied to ranges, squared ranges and the differences of squared ranges and further to pseudoranges, squared pseudoranges and the differences of pseudoranges.

## [01296] Robust Location Estimation in Wildlife Tracking Systems

**Format :** Talk at Waseda University

**Author(s) :** Sivan Toledo (Tel Aviv University)Eitam Arnon (Tel Aviv University)Shlomo Cain (Tel Aviv University)Assaf Uzan (Tel Aviv University)Ran Nathan (Hebrew University of Jerusalem)Orr Spiegel (Tel Aviv University)

**Abstract :** The talk will describe new location-estimation algorithms for time-of-arrival transmitter localization systems. The new algorithms use the consensus principle and they detect and discard outlier time-of-arrival observations, which

can be caused by non-line-of-sight propagation, radio interference, clock glitches, or an overestimation of the signal-to-noise ratio. They also detect cases in which two locations are equally consistent with the measurements and can usually select the correct one based on unambiguous estimates shortly before or after.

## [00581] Analysis, Methods and Applications in Complex Materials

### **Session Time & Room :**

00581 (1/2) : 5C (Aug.25, 13:20-15:00) @E603

00581 (2/2) : 5D (Aug.25, 15:30-17:10) @E603

### **Type :** Proposal of Minisymposium

**Abstract :** Materials modeling and simulation is essential in underpinning the discovery and synthesis of new materials and chemicals with novel functionalities in various key areas like energy and biomedicine. Materials science provides a rich source of problems in computational mathematics. Meanwhile, mathematicians are crucial to address fundamental questions with a solid theoretical foundation. The overarching goal of this minisymposium is to promote academic exchanges and collaborations among researchers working in the exciting and rapidly developing field of mathematics in materials science, especially focusing on the mathematical theory in complex materials as well as the applications of state-of-art machine-learning techniques.

**Organizer(s) :** Xiaoxu Li, Yangshuai Wang

**Classification :** 65G99, 81V70, 81V55

### **Minisymposium Program :**

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00581 (1/2) : 5C @E603 [Chair: Xiaoxu Li]

## [04090] A framework for a generalization analysis of MLIPs

### **Format :** Online Talk on Zoom

**Author(s) :** Yangshuai Wang (University of British Columbia)

**Abstract :** I will talk about an analytical (as opposed to statistical) approach to demonstrate the generalization of MLIPs and its application on simulating crystalline defects, explaining how the choice of training data and the accuracy of the fit to that training data affect the accuracy of predictions on materials properties.

## [04086] A Finite Element Configuration Interaction Method for Wigner Localization

### **Format :** Online Talk on Zoom

**Author(s) :** Xue Quan (Beijing Normal University)Huajie Chen (Beijing Normal University)

**Abstract :** This work proposes a numerical algorithm to study the Wigner localization phenomenon which carefully treats the many-body correlations. The main features are three-fold: (i) a finite element discretization of the one-body space such that the sharp localization can be captured; (ii) a good initial state obtained by exploiting the strongly correlated limit; and (iii) a selected configuration interaction method by choosing the Slater determinants from (stochastic) gradients.

## [05440] Equivariant Tensor Network Potentials

### **Format :** Talk at Waseda University

**Author(s) :** Max Hodapp (Materials Center Leoben)Alexander Shapeev (Skoltech)

**Abstract :** The computational cost of many state-of-the-art machine-learning interatomic (MLIPs) potentials increases exponentially with the number of atomic features. Low-rank tensor networks can overcome exponential growth in complexity, however, it is often not easy to encode the model symmetries. Here, we propose a formalism for rank-efficient equivariant tensor networks (ETNs) that remain invariant under actions of SO(3), and, using ETNs, develop a new class of MLIPs that demonstrate superior performance over existing MLIPs.

## [04136] Planewave approximation for electronic structure calculation of incommensurate systems

**Format :** Talk at Waseda University

**Author(s) :** Ting Wang (Academy of Mathematics and Systems Science, Chinese Academy of Sciences )

**Abstract :** Incommensurate structures come from stacking the single layers of low-dimensional materials on top of one another with misalignment, such as a twist in orientation. While these structures are of significant physical interest, they pose many theoretical challenges due to the loss of periodicity. Under the planewave framework, we provide a numerical scheme to compute the electronic structure of incommensurate systems based on density functional theory.

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00581 (2/2) : 5D @E603 [Chair: Ting Wang]

## [04088] DeePN2: A Deep Learning-Based Non-Newtonian Hydrodynamic Model

**Format :** Talk at Waseda University

**Author(s) :** Lidong Fang (Michigan State University)Pei Ge (Michigan State University)Lei Zhang (Shanghai Jiao Tong University)Weinan E (Peking University)Huan Lei (Michigan State University)

**Abstract :** A longstanding problem in the modeling of non-Newtonian hydrodynamics of polymeric flows is the availability of reliable and interpretable hydrodynamic models that faithfully encode the underlying microscale polymer dynamics. The main complication arises from the long polymer relaxation time, the complex molecular structure, and the heterogeneous interaction. DeePN2, a deep learning-based non-Newtonian hydrodynamic model, has been proposed and has shown some success in systematically passing the micro-scale structural mechanics information to the macro-scale hydrodynamics for suspensions with simple polymer conformation and bond potential. The model retains a multi-scaled nature by mapping the polymer configurations into a set of symmetry-preserving macro-scale features. The extended constitutive laws for these macro-scale features can be directly learned from the kinetics of their micro-scale counterparts. In this paper, we develop DeePN2 using more complex micro-structural models. We show that DeePN2 can faithfully capture the broadly overlooked viscoelastic differences arising from the specific molecular structural mechanics without human intervention.

## [04357] Numerical Analysis of Structural Green's Function in Multiple Scattering Theory

**Format :** Talk at Waseda University

**Author(s) :** Xiaoxu Li (Beijing Normal University)Huajie Chen (Beijing Normal University)

**Abstract :** This work studies the multiple scattering theory, also called Green's function method, in the electronic structure calculations of disordered systems from a mathematical perspective. By analyzing the structural Green's function, which can be viewed as the representation of Green's function in some basis, we will (a) improve the space truncation way to accelerate model convergence; (b) establish a mathematical analysis framework for Green's function and provide a prior error estimate; (c) design two linear-scaling algorithms with systematically controllable error.

## [04087] Variational Monte Carlo from a Continuous Viewpoint

**Format :** Talk at Waseda University

**Author(s) :** Juerong Feng (Beijing Normal University)Huajie Chen (Beijing Normal University)

**Abstract :** We study the variational Monte Carlo (VMC) method for quantum many-body problems based on data-driven wavefunction ansatz. We present a continuous stochastic gradient flow formulation for the VMC algorithm and show the large-time asymptotics with an explicit decay bound in terms of the many-body Hamiltonian and the wavefunction parameterization. In particular, we perform a careful analysis of the interactions between the approximation error of the ground state wavefunction and the generalization error of the sampling.

## [00584] Advanced Methods for Structured Eigenvalue Problems and Nonlinear Equations

**Session Time & Room :**

00584 (1/3) : 2D (Aug.22, 15:30-17:10) @E603

00584 (2/3) : 2E (Aug.22, 17:40-19:20) @E603

00584 (3/3) : 3C (Aug.23, 13:20-15:00) @E603

**Type :** Proposal of Minisymposium**Abstract :** Structured eigenvalue problems and nonlinear equations arise from many applications including 3D phononic crystals, medical image processing and phase retrieval. Their structure reflects certain physical properties that need to be preserved during calculations, posing a huge challenge for computational scientists. In recent years, many new methods and algorithms have been achieved, such as Jacobi–Davidson type algorithms, Newton-Noda iteration, GPR parameter prediction method, and multi-symplectic block-Lanczos methods. And theoretical analysis receives new progress on generalized orthogonal flow, nonlinear energy minimization and Davis-Kahan theorem. In this minisymposia, the invited speakers will present their recent advances about such interesting subjects.**Organizer(s) :** Zhigang Jia, Yanfei Jing, Yuan Lei, Tixiang Li**Classification :** 65F15, 65F45, 65F08, 65H17**Minisymposium Program :**

00584 (1/3) : 2D @E603

## **[01505] Eigen-decomposition and Fast Solvers for Maxwell's Equations for 3D Photonic Crystals**

**Format :** Talk at Waseda University**Author(s) :** Tixiang Li (Southeast University) Heng Tian (Sichuan University of Science and Engineering) Xing-Long Lyu (Southeast University) Wen-Wei Lin (National Yang Ming Chiao Tung University)**Abstract :** In this article, we propose the Fast Algorithms for Maxwell's Equations FAME package for solving Maxwell's equations for modeling three-dimensional photonic crystals. FAME combines the null-space free method with fast Fourier transform FFT-based matrix-vector multiplications to solve the generalized eigenvalue problems GEPs arising from the oblique Yee's discretization. Numerical results demonstrate the potential of our proposed package to enable large-scale numerical simulations for novel physical discoveries and engineering applications of photonic crystals.

## **[01246] Projected Gradient Method for Volume-Measure-Preserving Optimal Mass Transportation Problems**

**Format :** Talk at Waseda University**Author(s) :** Tsung-Ming Huang (National Taiwan Normal University) Wei-Hung Liao (National Yang Ming Chiao Tung University) Wen-Wei Lin (National Yang Ming Chiao Tung University) Mei-Heng Yueh (National Taiwan Normal University) Shing-Tung Yau (Tsinghua University)**Abstract :** Volumetric stretch energy minimization (VSEM) has been widely applied to the computation of volume-/mass-preserving parameterizations of simply connected tetrahedral mesh models. In this talk, based on the VSEM algorithm, we propose a projected gradient method for the computation of the volume/mass-preserving optimal mass transport map with a guaranteed convergence rate of  $O(1/m)$ . Numerical experiments are presented to justify the theoretical convergence behavior for various examples drawn from known benchmark models. Moreover, these numerical experiments show the effectiveness and accuracy of the proposed algorithm, particularly in the processing of 3D medical MRI brain images.

## **[01095] Multitask kernel-learning Gaussian process regression parameter prediction method and its application in matrix splitting iteration methods**

**Format :** Talk at Waseda University**Author(s) :** Juan Zhang (Xiangtan University)**Abstract :** In this talk, we present a multitask kernel-learning Gaussian process regression (GPR) parameter prediction method, and apply it in matrix splitting iteration methods. The first application is developing a general alternating direction implicit (ADI) framework, which can put most existing ADI methods into a unified framework and offer more new ADI approaches. Using the GPR method, the splitting parameter selection of this framework can be solved. The second application is for solving time-dependent linear systems, we give a new matrix splitting Kronecker product method, which can unify the existing Kronecker product schemes. Using the Multitask kernel-learning method, simultaneous multiple splitting parameters prediction and data-driven kernel learning can all be achieved. Based on Bayesian inference, the GPR method only requires a small training data set for learning the regression prediction mapping, and has sufficient accuracy and high generalization capability. We apply our developed methods to solving (time-dependent) convection-diffusion equations and (differential) Sylvester matrix equations. Numerical results illustrate our methods can solve large sparse linear systems more efficiently compared with existing methods.

## [01322] Breakdown Avoidance Structure-Preserving Doubling Algorithms for Nonlinear Matrix Equations

**Format :** Talk at Waseda University

**Author(s) :** Yueh-Cheng Kuo (National university of Kaohsiung)

**Abstract :** Structure-Preserving Doubling Algorithms (SDAs) are efficient algorithms for solving Riccati-type matrix equations. However, the breakdown may happen in the SDA. To avoid the breakdown, we first introduce the class of  $\Omega$ -symplectic forms,  $\Omega$ -SF, consisting of symplectic matrix pairs with Hermitian parametric matrix  $\Omega$ . Based on the  $\Omega$ -SF, we developed modified SDAs, called MSDAs, for solving the Riccati-type equations. The MSDA generates a sequence of symplectic matrix pairs in  $\Omega$ -SF and can avoid the breakdown by employing a suitable Hermitian matrix  $\Omega$ . In addition, we show that the Hermitian matrix  $\Omega$  in MSDAs can be chosen as a real diagonal matrix which can reduce the computational complexity. In this case, MSDA and SDA have the same computational complexity.

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00584 (2/3) : 2E @E603

## [01293] Newton-Noda iteration for nonlinear eigenvalue problems

**Format :** Talk at Waseda University

**Author(s) :** Ching-Sung Liu (National University of Kaohsiung)

**Abstract :** In this talk, we will introduce nonlinear eigenvalue problems, including tensor eigenvalue problems and nonlinear Schrödinger equations. We present a Newton-Noda iteration (NNI) to find positive eigenvectors of nonlinear problems. A great advantage of this method is that it converges quadratically and maintains positivity, i.e., the vector approximating the Perron vector (or ground state vector) is strictly positive in each iteration.

## [01584] Phase Retrieval of Quaternion Signal via Wirtinger Flow

**Format :** Talk at Waseda University

**Author(s) :** Junren Chen (University of Hong Kong) Michael Kwok-Po Ng (University of Hong Kong)

**Abstract :** Quaternion phase retrieval (QPR) is concerned with the recovery of quaternion signal from magnitude of quaternion linear measurements. We develop the scalable algorithm quaternion Wirtinger flow (QWF) for solving QPR, and establish its linear convergence guarantee. We develop a variant of QWF that can effectively utilize a pure quaternion priori by incorporating a quaternion phase factor estimate into QWF iterations.

## [01454] Numerical Methods for the Complete Solution of Multiparameter Eigenvalue Problems

**Format :** Online Talk on Zoom

**Author(s) :** Bo Dong (Dalian University of Technology)

**Abstract :** The linear/nonlinear multiparameter eigenvalue problems appear frequently in the study of multiparameter Sturm-Liouville problems and delay differential equations with some delays. In this talk, I will introduce two classes of numerical methods for solving the multiparameter eigenvalue problems: the method of transforming to simultaneous eigenvalue problems and the homotopy method. The former is suitable for small-scale and medium-scale problems while the latter tends to be more effective in terms of speed, accuracy and memory storage as the problem size grows. Numerical experiments and applications are presented to show the efficiency of these two classes of methods.

## [02763] Perturbation theory for the symmetry eigenvalue problem and singular value decomposition followed by deflation techniques

**Format :** Online Talk on Zoom

**Author(s) :** Xiang Wang (Nanchang University) Hongjia Chen (Nanchang University)

**Abstract :** The calculation of the dominant eigenvalues of a symmetric matrix  $A$  together with its eigenvectors, followed by the calculation of the deflation of  $A_1 = A - \rho U_k U_k^T$  corresponds to one step of the Wielandt deflation technique, where  $\rho$  is a shift and  $U_k$  are eigenvectors of  $A$ . In this paper, we investigate how the eigenspace of  $A_1$  changes when  $A_1$  is perturbed to  $\tilde{A}_1 = A - \rho \tilde{U}_k \tilde{U}_k^T$ ,  $\tilde{U}_k$  are approximate eigenvectors of  $U_k$ . We establish the bounds for the angle of eigenspaces of  $A_1$  and  $\tilde{A}_1$  based on the Davis-Kahan theorem.

Moreover, in the practical implementation for singular value decomposition, once one or several singular triplets converge to a preset accuracy, they should be deflated by  $B_1 = B - \gamma W_k V_k^H$  with  $\gamma$  is a shift and  $W_k$  and  $V_k$  are singular vectors so that they will not be re-computed.

We investigate how the singular subspaces of  $B_1 = B - \gamma W V^H$  changes when  $B_1$  is perturbed to  $\tilde{B}_1 = B - \gamma \tilde{W} \tilde{V}^H$ ,  $\tilde{W}$  and  $\tilde{V}^H$  are approximate singular vectors.

We also establish the bounds

for the angle of singular subspaces of  $B_1$  and  $\tilde{B}_1$  based on the Wedin theorem.

We show, by numerical experiment, the angles of eigenspaces and the angles of singular subspaces are well-predicted by these bounds with an appropriate shift.

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00584 (3/3) : 3C @E603

## [01112] Nonlinear Energy Minimization for Simplicial Manifold Parameterizations

**Format :** Talk at Waseda University

**Author(s) :** Mei-Heng Yueh (National Taiwan Normal University)

**Abstract :** The parameterization problem aims to efficiently compute a diffeomorphism between a simplicial manifold and a specified canonical domain. In this talk, I will introduce the theoretical and computational aspects of nonlinear energy minimization for the computation of parameterizations of simplicial manifolds that preserve the specified geometry property. Applications to manifold registration and image processing will be demonstrated to show the effectiveness of parameterizations.

## [01534] Two harmonic Jacobi–Davidson methods for computing a partial GSVD of a large matrix pair

**Format :** Talk at Waseda University

**Author(s) :** Jinzhi Huang (Soochow University)Zhongxiao Jia (Tsinghua University)

**Abstract :** Two harmonic extraction-based Jacobi–Davidson (JD) type algorithms are proposed to compute a partial generalized singular value decomposition (GSVD) of a large regular matrix pair. They are called cross product-free (CPF) and inverse-free (IF) harmonic JDGSVD algorithms, abbreviated as CPF-HJDGSVD and IF-HJDGSVD, respectively. Compared with the standard extraction-based JDGSVD algorithm, the harmonic extraction-based algorithms converge more regularly and suit better for computing GSVD components corresponding to interior generalized singular values. Thick-restart CPF-HJDGSVD and IF-HJDGSVD algorithms with some deflation and purgation techniques are developed to compute more than one GSVD components. Numerical experiments confirm the superiority of CPF-HJDGSVD and IF-HJDGSVD to the standard extraction-based JDGSVD algorithm.

## [01473] Harmonic multi-symplectic Lanczos algorithm for quaternion singular triplets

**Format :** Talk at Waseda University

**Author(s) :** XUAN LIU (University of Macau)Zhigang Jia (Jiangsu Normal University)Jingfei Zhu (Jiangsu Normal University)Meixiang Zhao (Jiangsu Normal University)

**Abstract :** The computation of quaternion singular triplets has become one of the core targets of color image processing. A novel harmonic multi-symplectic Lanczos algorithm is presented for approximating extreme quaternion singular triplets. The underlying theory is to preserve an algebraic structure during the partial bidiagonalization, the argumentation, and the restarted bidiagonalization. The proposed algorithm is successfully applied to color video semantic segmentation.

## [01319] The asymptotic analysis of generalized orthogonal flows

**Format :** Talk at Waseda University

**Author(s) :** Shih-Feng Shieh (National Taiwan Normal University)

**Abstract :** This talk is concerned with the matrix differential equation approximating the k-dimensional dominant eigenspace of a matrix. The solution of the matrix differential equation is orthogonal and is called generalized orthogonal flow. The existence and uniqueness of the generalized orthogonal flow are guaranteed for all time  $t \in \mathbb{R}$ . An orthogonal flow, which has the shortest arc-length, has been constructed and is called the best path of generalized orthogonal flows. We show that the best path is Oja's flow. We also analyze the asymptotic behaviors and the convergence rate of the best path.

# [00586] Challenges for Attaining High-performance in Numerical Software

**Session Time & Room :** 3D (Aug.23, 15:30-17:10) @E603

**Type :** Proposal of Minisymposium

**Abstract :** The architectures of the existing top performing systems are undeniable complex, building upon multi-core units and proprietary interconnects, with very high levels of parallelism. These features pose many challenges to numerical library and application developers. In addition, accuracy of numerical computations, which can be an issue for conventional (e.g., BLAS) or complex algorithms (e.g., eigensolvers), should be concerned. In this minisymposium will discuss recent work on Automatic tuning (AT) by using expandable AI, novel approaches for accuracy verification, and iterative eigensolvers that do not enforcing orthogonality on the iterates thus reducing communication.

**Organizer(s) :** Takahiro Katagiri, Osni Marques, Toshiyuki Imamura

**Classification :** 65F15, 68T99, 68U99, 65G99, 65F05, Auto-tuning

**Minisymposium Program :**

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00586 (1/1) : 3D @E603 [Chair: Takahiro Katagiri]

## [03413] Adaptation of XAI to Numerical Libraries: A Case Study for Automatic Performance Tuning

**Format :** Talk at Waseda University

**Author(s) :** Takahiro Katagiri (Nagoya University)

**Abstract :** AI is one of crucial technologies. On the other hand, we have been adapting to auto-tuning (AT) for numerical software. By utilizing AI technology, it is expected to establish AT function for performance tuning on numerical libraries. However, it is difficult to verify correctness for obtained AI model. Adaptation of explainable AI (XAI) is one of solutions. In this presentation, several scenarios for adapted XAI to AT function will be demonstrated.

## [03472] Parallel Eigensolvers Based on Minimization Strategies

**Format :** Talk at Waseda University

**Author(s) :** Doru Thom Popovici (Lawrence Berkeley National Lab)Osni Marques (Lawrence Berkeley National Laboratory)Mauro Del Ben (Lawrence Berkeley National Laboratory)Andrew Canning (Lawrence Berkeley National Laboratory)

**Abstract :** This presentation will show recent developments in unconstrained minimization strategies for the solution of eigenvalue problems in electronic structure calculations. These schemes employ a preconditioned conjugate gradient approach that avoids an explicit reorthogonalization of the trial eigenvectors, in contrast to typical iterative eigensolvers, therefore reducing communications and becoming an attractive approach for the solution of very large problems on massively parallel computers. The presentation will also discuss the need to rearrange calculations (sometimes counteractively) to achieve performance, in particular on GPUs.

## [03700] Mixed-precision iterative refinement for real-symmetric eigenvalue decomposition with clustered eigenvalues

**Format :** Talk at Waseda University

**Author(s) :** Yuki Uchino (Shibaura Institute of Technology)Katsuhisa Ozaki (Shibaura Institute of Technology)Toshiyuki Imamura (RIKEN)

**Abstract :** Uchino et al. presented two mixed-precision iterative refinement algorithms (herein called Algorithm 1 and 2) for the real-symmetric eigendecomposition based on the algorithm proposed by Ogita and Aishima.

Algorithm 2 offers the same convergence and advantages in terms of computational speed compared to Algorithm 1, as demonstrated through numerical experiments on the supercomputer Fugaku housed at RIKEN R-CCS.

We will also show that Algorithm 2 is much faster than the eigensolver provided in ScaLAPACK.

## [04170] Mixed Precision Iterative Refinement with H-matrices

**Format :** Talk at Waseda University

**Author(s) :** Thomas Spendhofer (Tokyo Institute of Technology)Rio Yokota (Tokyo Institute of Technology)

**Abstract :** It has been shown that the solution to a dense linear system can be accelerated by using mixed precision iterative refinement relying on approximate LU-factorization.

We investigate the usage of both mixed precision and low-rank approximations for obtaining an approximate

factorization. When employing the hierarchical matrix format, we are able to attain results accurate to a double precision solver at a lower complexity of  $\text{order}n^2$  for certain matrices.

## [00587] Recent Advances in Numerical Methods for Nonlinear Hyperbolic PDEs

### **Session Time & Room :**

00587 (1/2) : 2D (Aug.22, 15:30-17:10) @D401

00587 (2/2) : 2E (Aug.22, 17:40-19:20) @D401

**Type :** Proposal of Minisymposium

**Abstract :** Numerically solving hyperbolic systems of conservation and balance laws is a challenging task as their solutions may develop extremely complicated nonsmooth structures. The number of applications in which such systems arise keeps increasing and most of the existing methods have their restrictions and disadvantages. Therefore, it is extremely important to develop new, highly accurate, stable, and robust numerical methods. The mini-symposium will focus on recent developments in this field of research and will bring together researchers from different countries and provide an opportunity for in-depth scientific discussion and exchange of ideas on the development, analysis, and applications of modern methods.

**Organizer(s) :** Alina Chertock, Alexander Kurganov

**Classification :** 76M12, 76M20, 76M10, 35L65, 35L67

### **Minisymposium Program :**

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00587 (1/2) : 2D @D401 [Chair: Alexander Kurganov]

## [01485] A New Locally Divergence-Free Path-Conservative Central-Upwind Scheme for Ideal and Shallow Water Magnetohydrodynamics

**Format :** Talk at Waseda University

**Author(s) :** Alina Chertock (North Carolina State University)Alexander Kurganov (Southern University of Science and Technology)Michael Redle (North Carolina State University)Kailiang Wu (Southern University of Science and Technology)

**Abstract :** This talk presents a new second-order unstaggered path-conservative central-upwind scheme for ideal and shallow water MHD equations. The new scheme locally preserves the divergence-free constraint, does not rely on Riemann problem solvers, and robustly produces high-resolution and non-oscillatory results. The derivation of the scheme is based on the Godunov-Powell nonconservative modifications of the studied systems and by augmenting it with the evolution equations for the corresponding derivatives of the magnetic field components.

## [01517] Geometric Quasilinearization (GQL) for Bound-Preserving Schemes of Hyperbolic PDEs

**Format :** Talk at Waseda University

**Author(s) :** Kailiang Wu (Southern University of Science and Technology)Chi-Wang Shu (Brown University)

**Abstract :** Solutions to many partial differential equations satisfy certain bounds or constraints. For example, the density and pressure are positive for equations of fluid dynamics, and in the relativistic case the fluid velocity is upper bounded by the speed of light, etc. As widely realized, it is crucial to develop bound-preserving numerical methods that preserve such intrinsic constraints. Exploring provably bound-preserving schemes has attracted much attention and is actively studied in recent years. This is however still a challenging task for many systems especially those involving nonlinear constraints.

Based on some key insights from geometry, we systematically propose a novel and general framework, referred to as geometric quasilinearization (GQL), which paves a way for studying bound-preserving problems with nonlinear constraints. The essential idea of GQL is to equivalently transfer all nonlinear constraints into linear ones, through properly introducing some free auxiliary variables. We establish the fundamental principle and general theory of GQL via the geometric properties of convex regions, and propose three simple effective methods for constructing GQL. We apply the GQL approach to a variety of partial differential equations, and demonstrate its effectiveness and remarkable advantages for studying bound-preserving schemes, by diverse challenging examples and applications which cannot be easily handled by direct or traditional approaches.

## [01722] An improved non-hydrostatic shallow-water type model for the simulation of landslide generated tsunamis

**Format :** Talk at Waseda University

**Author(s) :** Manuel J Castro Diaz (University of Málaga)Tomas Morales de Luna (Universidad de Malaga)Cipriano Escalante Sanchez (Universidad de Málaga)Jorge Macías Sanchez (University of Málaga)Enrique D Fernandez Nieto (University of Sevilla)

**Abstract :** In this talk we present an improved version of a non-hydrostatic shallow-water system coupled with a granular landslide shallow-water type model for the numerical simulation of tsunamis generated by landslides. The system is discretized by means of a high-order WB finite volume scheme. Some numerical tests with laboratory experiments and real events will be presented to show the capabilities of the proposed model.

## [01949] A New Approach for Designing Well-Balanced Schemes for the Shallow Water Equations

**Format :** Talk at Waseda University

**Author(s) :** Remi Abgrall (University of Zurich)Yongle Liu (University of Zurich)

**Abstract :** In this talk, I will introduce a new approach for constructing robust well-balanced numerical methods for one-dimensional Saint-Venant system. We combine the conservative and non-conservative formulations of the studied hyperbolic system in a natural way. The solution is globally continuous and described by a combination of point values and average values, which will be evolved by two different forms of PDEs. We demonstrate the behavior of the new scheme on a number of challenging examples.

00587 (2/2) : 2E @D401 [Chair: Alina Chertock]

## [02636] Error analysis of finite volume methods for the Euler equations via relative energy

**Format :** Talk at Waseda University

**Author(s) :** Maria Lukacova (University of Mainz)Bangwei She (Capital Normal University)Yuhuan Yuan (University of Mainz)

**Abstract :** We present an overview of our recent results for the error analysis of some finite volume methods for multidimensional Euler system. To control global error, we apply the relative energy principle and estimate the L2 norm between a numerical solution and the strong solution.

If time permits, we will present an extension to the error analysis of the random Euler system approximated by the Monte Carlo finite volume method.

## [04782] Flux Globalization Based Well-Balanced Path-Conservative Central-Upwind Schemes

**Format :** Talk at Waseda University

**Author(s) :** Alexander Kurganov (Southern University of Science and Technology)

**Abstract :** The talk will focus on numerical methods for nonconservative hyperbolic systems of balance laws. I will introduce well-balanced path-conservative central-upwind schemes, which are based on the flux globalization: both source and nonconservative product terms are incorporated into the global flux. The resulting quasi-conservative system is numerically solved using a semi-discrete central-upwind scheme with the numerical fluxes are evaluated using the path-conservative technique. Applications to several shallow water models will be demonstrated.

## [01953] High order well-balanced and asymptotic preserving WENO schemes for the shallow water equations

**Format :** Online Talk on Zoom

**Author(s) :** Yulong Xing (Ohio State University)

**Abstract :** Shallow water equations (SWEs) with a non-flat bottom topography have been widely used to model flows in rivers and coastal areas. In this presentation, we will talk about the applications of high-order semi-implicit well-balanced and asymptotic preserving (AP) WENO methods to this system. We consider the Froude number ranging from O(1) to 0, which in the zero Froude limit becomes the “lake equations” for balanced flow without gravity waves. We apply a well-balanced finite difference WENO reconstruction, coupled with a stiffly accurate implicit-explicit (IMEX) Runge-Kutta time discretization. The resulting semi-implicit scheme can be shown to be well-balanced, AP and asymptotically accurate at the same time. Both one- and two-dimensional numerical results are provided to demonstrate the high order accuracy, AP property and good performance of the proposed methods in capturing small perturbations of steady state solutions.

# [00589] Computational Biomedical Physics and Mechanics

**Session Time & Room :**

00589 (1/2) : 5B (Aug.25, 10:40-12:20) @D514

00589 (2/2) : 5C (Aug.25, 13:20-15:00) @D514

**Type :** Proposal of Minisymposium

**Abstract :** Computational methods play a fundamental role in modern science and health research. This symposium is aimed to provide a platform to get computational experts to share recent simulation efforts in areas of biomedical physics and mechanics. The topics include but are not limited to biomedical fluid dynamics, treatment planning and computational surgery, anatomical modeling from medical imaging, multi-physics modeling of biological processes, medical acoustics applied to hyperthermia and focused ultrasound therapy, ion channels/transporters study by continuum models, kinetic models and molecular dynamics.

**Organizer(s) :** Tzyy-Leng Horng, Maxim Solovchuk

**Classification :** 92C05, 92C10, 92C30, 92C35, 92C50

**Minisymposium Program :**


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00589 (1/2) : 5B @D514 [Chair: Tzyy-Leng Horng]

## [01471] A Multi-Scale Approach to Model K+ Permeation Through the KcsA Channel

**Format :** Talk at Waseda University

**Author(s) :** Tzyy-Leng Horng (Feng Chia University)Ren-Shiang Chen (Tunghai University)Maria Vittoria Leonardi (University of Perugia)Fabio Franciolini (University of Perugia)Luigi Catacuzzeno (University of Perugia)

**Abstract :** K<sup>+</sup> channels allow a very efficient passage of K<sup>+</sup> ions through the membrane while excluding Na<sup>+</sup> ions, which is essential for life. The 3D structure of the KcsA K<sup>+</sup> channel allows to address many relevant aspects of K<sup>+</sup> permeation and selectivity mechanisms at the molecular level. Using a multi-scale approach, we studied the mechanism of K<sup>+</sup> permeation through KcsA channels and reproduced the main permeation properties of the KcsA channel found experimentally.

## [02551] Modeling electrohydrodynamic flow through a nanochannel

**Format :** Talk at Waseda University

**Author(s) :** Kumar Saurabh (National Health Research Institutes)Maxim A Solovchuk (National Health Research Institutes)

**Abstract :** Fluid-ion transport through a nanochannel can be described through coupled fourth order-Poisson-Nernst-Planck-Bikerman (4PNPBik) and Navier-Stokes equations. The 4PNPBik model describes ionic and nonionic interactions between particles while accounting for the effect of polarization of the medium, electrostatic correlations, solvation of ions etc. Navier-Stokes equations model the hydrodynamics of the system. Governing equations are discretized using lattice Boltzmann method on GPU. Impact of phenomenon like viscoelectric effect, finite size of particles, velocity slip, non-homogeneous diffusion etc. has been studied.

## [02740] Double diffusion for nanofluid

**Format :** Talk at Waseda University

**Author(s) :** Yende Chou (National Taiwan University)Maxim A Solovchuk (National Health Research Institutes)Wei-Shien Hwang (National Taiwan University)

**Abstract :** In double diffusion problems, fluid is driven by temperature and concentration differences within the flow field. By adding nanoparticles into the fluid to form a nanofluid, heat transfer and mass transfer can be enhanced. This study investigates the effect of volume fraction of nanoparticles on heat and mass transfer in a three-dimensional square cavity. The governing equations for this problem are mass conservation, momentum conservation, energy conservation and mass transfer equations. The finite volume method is applied to discretize these equations. Multigrid method is developed for the solution of flow problem to improve computational efficiency.

## [03003] GPU Computation of High-Intensity Focused Ultrasound Ablation Under Different Pathways

**Format :** Talk at Waseda University

**Author(s) :** Tatiana Filonets (National Taiwan University)Maxim Solovchuk (National Health Research Institutes)

**Abstract :** High-performance computing is important to accelerate the numerical solutions of partial differential equations which are used for modeling high-intensity focused ultrasound and temperature.

The nonlinear Westervelt equation was coupled with the bioheat equation to model temperature under ultrasound sonication. CUDA program was developed for GPU to speed up computations.

An appropriate scanning pathway can help to ablate a big tumor volume uniformly within a few minutes considering that cavitation can also affect the lesion form.

00589 (2/2) : 5C @D514

## [00592] Optimization and Inverse Problems

**Session Time & Room :**

00592 (1/2) : 1C (Aug.21, 13:20-15:00) @A207

00592 (2/2) : 1D (Aug.21, 15:30-17:10) @A207

**Type :** Proposal of Minisymposium

**Abstract :** In an inverse problem, we want to come up with a good description of a phenomenon from bad measurements. Industrial-scale inverse problems include, in particular, medical and biological imaging, structural health monitoring, and process monitoring. Generally the inverse problem takes the form of an ill-posed operator equation, linear or nonlinear. To solve such a problem, often the problem is given a variational formulation to which regularisation is added to promote desirable solution features. The solution of the inverse problem then becomes dependent on efficient optimisation methods. The talks in this minisymposium cover recent research in the area. They present general-purpose optimisation algorithms and numerical techniques, and the application of such methods to inverse problems.

**Organizer(s) :** Tuomo Valkonen, Elena Resmerita

**Classification :** 90C30, 65K10, 92C55, Inverse problems, optimisation, nonsmooth optimisation

**Minisymposium Program :**

00592 (1/2) : 1C @A207 [Chair: Elena Resmerita]

## [03137] Sparsity-promoting regularization for inverse problems via statistical learning

**Format :** Talk at Waseda University

**Author(s) :** Luca Ratti (University of Bologna)Giovanni S Alberti (University of Genoa)Ernesto De Vito (University of Genoa)Tapio Helin (Lappeenranta-Lahti University of Technology)Matti Lassas (University of Helsinki)Matteo Santacesaria (University of Genoa)

**Abstract :** In this talk, I will discuss a strategy, based on statistical learning, to design variational regularization functionals for ill-posed linear inverse problems. The proposed approach first restricts the choice to a parametric class of functionals and then searches for the optimal regularizer inside it, combining model-based and data-driven information. I will first recap the main results in the case of generalized Tikhonov functionals, and then focus on a class of sparsity-promotion regularizers.

## [03391] Online Optimization for Dynamic Electrical Impedance Tomography

**Format :** Talk at Waseda University

**Author(s) :** Jyrki Jauhainen (University of Helsinki)Tuomo Valkonen (Escuela Politécnica Nacional)Neil Dizon (University of Helsinki)

**Abstract :** Online optimization generally studies the convergence of optimization methods as more data is introduced into the problem; think of deep learning as more training samples become available. We adapt the idea to dynamic inverse problems that naturally evolve in time. We introduce an improved primal-dual online method specifically suited to these problems, and demonstrate its performance on dynamic monitoring of electrical impedance tomography.

## [03177] Primal-Dual Methods with Adjoint Mismatch

**Format :** Talk at Waseda University

**Author(s) :** Felix Schnepp (Technische Universität Braunschweig)

**Abstract :** Primal-dual algorithms are widespread methods to solve saddle-point problems of the form  $\min_x \max_y G(x) + \langle Ax, y \rangle - F^*(y)$ . However, in practical applications like computed tomography the adjoint operator is often replaced by a computationally more efficient approximation. This leads to an adjoint mismatch in the algorithm.

In this talk, we analyse the convergence of different primal-dual algorithms and prove conditions, under which the existence of a solution can still be guaranteed.

## [02036] Material decomposition in multi-energy X-Ray tomography with Inner Product Regularizer

**Format :** Online Talk on Zoom

**Author(s) :** Salla Maaria Latva-Äijö (University of Helsinki)

**Abstract :** Dual-energy X-ray tomography is considered in a context where the target under imaging consists of two or more distinct materials. The materials are assumed to be possibly intertwined in space, but at any given location there is only one material present. Further, the same number of X-ray energies are chosen so that there is a clear difference in the spectral dependence of the attenuation coefficients of the materials.

A novel regularizer is presented for the inverse problem of reconstructing separate tomographic images for the two materials. A combination of two things, (a) non-negativity constraint, and (b) penalty term containing the inner product between the two material images, promotes the presence of at most one material in a given pixel. A preconditioned interior point method is derived for the minimization of the regularization functional.

Numerical tests with digital phantoms suggest that the new algorithm outperforms the baseline method, Joint Total Variation regularization, in terms of correctly material-characterized pixels. While the method is tested only in a two-dimensional setting with two materials and two energies, the approach readily generalizes to three dimensions and more materials. The number of materials just needs to match the number of energies used in imaging.

00592 (2/2) : 1D @A207 [Chair: Tuomo Valkonen]

## [05012] Multiscale hierarchical decomposition methods for ill-posed problems

**Format :** Talk at Waseda University

**Author(s) :** Tobias Wolf (Klagenfurt University)Elena Resmerita (University of Klagenfurt)Stefan Kindermann (Johannes Kepler University Linz)

**Abstract :** The Multiscale Hierarchical Decomposition Method (MHDM) is a popular iterative method based on total variation minimization for mathematical imaging. We consider the method in a more general framework and expand existing results to the case when some classes of convex and nonconvex penalties are employed. Moreover, we discuss conditions under which the iterates of the MHDM agree with solutions of Tikhonov regularization corresponding to suitable regularization parameters. We illustrate our results with numerical examples.

## [05199] Multiscale hierarchical decomposition methods for images corrupted by multiplicative noise

**Format :** Talk at Waseda University

**Author(s) :** Elena Resmerita (University of Klagenfurt)Joel Barnett (UCLA)Wen Li (Fordham University)Luminita Vese (UCLA)

**Abstract :** Recovering images corrupted by multiplicative noise is a well known challenging task. Motivated by the success of multiscale hierarchical decomposition methods (MHDM) in image processing, we adapt a variety of both classical and new multiplicative noise removing models to the MHDM form. Theoretical and numerical results show that the MHDM techniques are effective in several situations.

## [03502] A Lifted Bregman Formulation for the Inversion of Deep Neural Networks

**Format :** Talk at Waseda University

**Author(s) :** Xiaoyu Wang (University of Cambridge)Martin Benning (Queen Mary University of London, London)

**Abstract :** We propose a novel framework for the regularised inversion of deep neural networks. The framework is based on the authors' recent work on the lifted Bregman formulation on training feed-forward neural networks without the differentiation of activation functions. We propose a family of variational regularisations based on Bregman distances,

present theoretical results and support their practical application with numerical examples. In particular, we present the first convergence result (to the best of our knowledge) for the regularised inversion of a single-layer perceptron that only assumes that the solution of the inverse problem is in the range of the regularisation operator, and that shows that the regularised inverse provably converges to the true inverse if measurement errors converge to zero.

### [03398] Stable Phase retrieval with mirror descent

**Format :** Online Talk on Zoom

**Author(s) :** Jean-Jacques Godeme (Normandie Univ, ENSICAEN, CNRS, GREYC, France)Jalal Fadili (Normandie Univ, ENSICAEN, CNRS, GREYC)Myriam Zerrad (Aix-Marseille Univ, CNRS, Centrale Marseille, Institut Fresnel, Marseille)Claude Amra (Aix-Marseille Univ, CNRS, Centrale Marseille, Institut Fresnel, Marseille)

**Abstract :** We aim to reconstruct an  $n$ -dimensional real vector from  $m$  phaseless measurements corrupted by additive noise. We use the mirror descent (or Bregman gradient descent) algorithm to deal with noisy measurements and prove that the procedure is robust to (small enough) noise.

## [00593] Advances in Nonlinear Dynamics

**Session Time & Room :**

00593 (1/3) : 1C (Aug.21, 13:20-15:00) @F308

00593 (2/3) : 1D (Aug.21, 15:30-17:10) @F308

00593 (3/3) : 1E (Aug.21, 17:40-19:20) @F308

**Type :** Proposal of Minisymposium

**Abstract :** The aim of dynamical systems theory is to understand the long term behavior of large sets of initial conditions, often for highly nonlinear models coming from realistic application problems. Due to the importance of nonlinear models, numerical calculations have long played an important role. In this session we bring together experts to discuss problems at the frontiers of our understanding. Some talks will focus on new computational methods, some on attempts to understand more and more realistic models, and some on theoretical issues which inform our approach to computational dynamics.

**Organizer(s) :** Evelyn Sander, Jason Mireles James

**Classification :** 37C05

**Minisymposium Program :**

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00593 (1/3) : 1C @F308

### [02779] Polynomial discretisations of transfer and Koopman operators in chaotic dynamics

**Author(s) :** Caroline Wormell (The Australian National University)

**Abstract :** Many long-term statistical properties of chaotic systems are encoded by transfer or Koopman operators. Orthogonal polynomial-based operator discretisations are generally very efficient, and I will show in expanding dynamics these operators are no exception: a Chebyshev discretisation allows fast, very accurate, rigorous estimates of expanding dynamics, even with parabolic fixed points. Furthermore, a theoretical extension to general orthogonal polynomials proves fast convergence of Extended Dynamical Mode Decomposition, a data-driven algorithm commonly used across physical sciences.

### [03719] Estimating the spectra for annealed transfer operators of random dynamical systems

**Author(s) :** Alex Blumenthal (Georgia Tech)Isaia Nisoli (Universidade Federal de Rio de Janeiro)Toby Taylor-Crush (University of Loughborough)

**Abstract :** I will describe some recent efforts with my collaborators Toby Taylor-Crush and Isaia Nisoli towards the computer-validated estimation of spectra for annealed transfer operators of random dynamical systems. Applications include the study of various stochastic bifurcations associated to the explosion of the support of a stationary measure as some underlying parameter is varied.

**[03734] Energy growth in Hamiltonian systems with small dissipation****Author(s)** : Marian Gidea (Yeshiva University)

**Abstract** : We consider a model for an energy harvesting device consisting of a rotator and a pendulum subject to a small perturbation given by a time-periodic Hamiltonian vector field plus a conformally symplectic vector field. In general, the system has energy dissipation. We provide explicit conditions so that the system exhibits energy growth. In theory, this shows Arnold diffusion in Hamiltonian systems with small dissipation. In practice, this translates into continuous generation of electricity.

**[03874] A dynamical systems approach to low-damage seismic design****Author(s)** : Hinke M Osinga (University of Auckland)

**Abstract** : An example of low-damage seismic design is the post-tensioned moment-resisting frame, which exhibits geometric nonlinearity under large deformations. Whether the tilt angle of the frame exceeds a prescribed maximum depends on the forcing properties. We show that this failure boundary is organised by so-called grazing orbits, which reach but do not move beyond the design limit of the frame. We consider both harmonic and aperiodic waves with a broader frequency content.

00593 (2/3) : 1D @F308

**[03886] Understanding how blenders emerge: weaving a carpet from global manifolds****Author(s)** : Dana C'Julio (University of Auckland)Bernd Krauskopf (University of Auckland)Hinke M Osinga (University of Auckland)

**Abstract** : A blender is a tool for constructing 'wild' robust chaotic dynamics in partially hyperbolic systems. We make precise statements about how a blender emerges in a family of 3D Hénon-like maps as parameters are changed. To this end, we employ advanced numerical techniques to determine when the one-dimensional stable manifolds of two saddle points weave through phase space to form an impenetrable carpet, which is the characterising property of a blender.

**[03948] A Dynamical Systems Approach for Most Probable Escape Paths over Periodic Boundaries****Author(s)** : Emmanuel Fleurantin (George Mason University, University of North Carolina at Chapel Hill)Katherine Slyman (University of North Carolina at Chapel Hill)Blake Barker (Brigham Young University)Christopher K.R.T. Jones (George Mason University, University of North Carolina at Chapel Hill)

**Abstract** : Analyzing when noisy trajectories, in the two dimensional plane, of a stochastic dynamical system exit the basin of attraction of a fixed point is specifically challenging when a periodic orbit forms the boundary of the basin of attraction. Our contention is that there is a distinguished Most Probable Escape Path (MPEP) crossing the periodic orbit which acts as a guide for noisy escaping paths in the case of small noise slightly away from the limit of vanishing noise. It is well known that, before exiting, noisy trajectories will tend to cycle around the periodic orbit as the noise vanishes, but we observe that the escaping paths are stubbornly resistant to cycling as soon as the noise becomes at all significant. Using a geometric dynamical systems approach, we isolate a subset of the unstable manifold of the fixed point in the Euler-Lagrange system, which we call the River. Using the Maslov index we identify a subset of the River which is comprised of local minimizers. The Onsager-Machlup (OM) functional, which is treated as a perturbation of the Friedlin-Wentzell functional, provides a selection mechanism to pick out a specific MPEP. Much of this talk will be focused on the system obtained by reversing the van der Pol Equations in time (so-called IVDP). Through Monte-Carlo simulations, we show that the prediction provided by OM-selected MPEP matches closely the escape hatch chosen by noisy trajectories at a certain level of small noise.

**[04096] On the connectedness and disconnectedness of the Julia set for the Hénon map.****Author(s)** : Zin Arai (Tokyo Institute of Technology)

**Abstract** : We discuss the connectedness and disconnectedness of the Julia set for the complex Hénon map. To prove the disconnectedness of the Julia set, we develop a topological method that uses the plurisubharmonic nature of the Green function. We also construct a hyperbolic complex Hénon map with a connected Julia set. Consequently, we obtain a certain topological property of the connectedness locus of the map. This is a joint work with Yutaka Ishii (Kyushu University).

## [04135] Standard piecewise smooth symplectic maps

**Author(s)** : Vered Rom-Kedar (The Weizmann Institute)Michal Pnueli (The Weizmann Institute)Alexandra Zobova (The Weizmann Institute)

**Abstract** : Return maps of near integrable/near quasi-integrable Hamiltonian impact systems are shown to produce piecewise smooth symplectic maps. In the integrable/quasi-integrable limit, these maps reduce to piecewise smooth families of rotations/interval exchange maps. As for the standard map, we introduce simplified models for these return maps and study their dynamics numerically. Regular and singular resonances emerge, as well as transient behavior, leading to conjectures regarding the non-existence of dividing circles in the singularity bands.

00593 (3/3) : 1E @F308

## [04300] Optimal linear response for expanding circle maps

**Author(s)** : Gary Froyland (UNSW Sydney)Stefano Galatolo (University of Pisa)

**Abstract** : We consider the problem of optimal linear response for deterministic expanding maps of the circle. To each infinitesimal perturbation of a circle map we consider the response of the expectation of an observation function, and the response of isolated spectral points of the transfer operator. Under mild conditions on the set of feasible perturbations we show there is a unique optimal perturbation. We derive expressions for the unique optimum, and devise a Fourier-based computational scheme.

## [04937] Finite element approximated manifolds for PDEs by the parameterization method

**Author(s)** : Jorge Gonzalez (Georgia Tech)Jason Desmonde Mireles James (Florida Atlantic University)Necibe Tuncer (Florida Atlantic University)

**Abstract** : The computation of invariant manifolds for PDEs is significantly challenging over irregular high dimensional domains where the classical Fourier methods are not applicable. This work presents a new framework of interest for practical applications that combines the parameterization method with the classical finite element method. We implement the method for a variety of examples having both polynomial and non-polynomial nonlinearities, on non-convex and not necessarily simply connected polygonal domains.

## [05240] Dynamics of a Hill four-body problem with oblate bodies

**Author(s)** : Wai Ting Lam (Florida Atlantic University)

**Abstract** : Consider a restricted four body problem with three oblate massive bodies, which are assumed to move in a plane under their mutual gravity, and an infinitesimal fourth body to move in the 3-dimensional space under the gravitational influence of the three heavy bodies, but without affecting them. By performing Hill approximation, we study the dynamics and properties of the infinitesimal body in a neighborhood of the smaller body.

## [05259] Parametrisation method for large finite element models of engineering structures

**Author(s)** : Alessandra Vizzaccaro (University of Exeter)Andrea Opreni (Politecnico di Milano)Giorgio Gobat (Politecnico di Milano)Attilio Alberto Frangi (Politecnico di Milano)Cyril Touze' (ENSTA Paris )

**Abstract** : In this contribution we present a method to directly compute asymptotic expansion of invariant manifolds of large finite element models from physical coordinates and their reduced order dynamics on the manifold. The focus of the talk is on engineering structures, whose spectrum around the fixed point is usually composed of complex conjugate pair of eigenvalues with always negative but small real part. This gives rise to rich dynamical behaviour such as internal resonances, parametric resonances, and superharmonic resonances. The accuracy of the reduction on the slow invariant manifold will be shown on selected examples.

## [00595] Combinatorial topological dynamics

**Session Time & Room :**

00595 (1/3) : 5B (Aug.25, 10:40-12:20) @G802

00595 (2/3) : 5C (Aug.25, 13:20-15:00) @G802

00595 (3/3) : 5D (Aug.25, 15:30-17:10) @G802

**Type :** Proposal of Minisymposium

**Abstract :** Recent years have seen the rapid development of topological data analysis. Via combinatorial modeling of space, TDA enables the study of the geometry of data using persistent homology. In particular, it may be used to analyze the phase space of a sampled dynamical system, thereby providing a static image. To get a dynamic view, a better understanding of classical topological tools in dynamics in the context of data is needed. The aim of this session is to bring together researchers from TDA and dynamical systems to study dynamic aspects of data via topological tools, in particular Morse and Conley theory.

**Organizer(s) :** Konstantin Mischaikow, Marian Mrozek, Thomas Wanner

**Classification :** 37B30, 37B35, 37E15, 57M99, 57Q05

**Minisymposium Program :**

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00595 (1/3) : 5B @G802 [Chair: Konstantin Mischaikow]

## [05133] Analyzing Network Representations of Dynamical Systems Using Persistent Homology

**Format :** Online Talk on Zoom

**Author(s) :** Elizabeth Munch (Michigan State University)

**Abstract :** Persistent homology, the flagship method of topological data analysis, can be used to provide a quantitative summary of the shape of data. One way to pass data to this method is to start with a finite, discrete metric space (whether or not it arises from a Euclidean embedding) and to study the resulting filtration of the Rips complex. In this talk, we will discuss several available methods for turning a time series into a discrete metric space, including the Takens embedding, and ordinal partition networks. Combined with persistent homology and machine learning methods, we show how this can be used to classify behavior in time series in both synthetic and experimental data.

## [01382] Topological Data Analysis of Spatiotemporal Honeybee Aggregation

**Format :** Online Talk on Zoom

**Author(s) :** Elizabeth Bradley (University of Colorado)Chad Topaz (Williams College)Golnar Gharooni Fard (University of Colorado)Varad Deshmukh (University of Colorado)Orit Peleg (University of Colorado)Morgan Byers (University of Colorado)

**Abstract :** We employ topological data analysis to explore honeybee aggregations in the context of trophallaxis: the exchange of food among nestmates.

Using synthetic and laboratory data, we build topological summaries called CROCKER plots to capture the shape of the data as a function of both scale and time. Our results show two distinct regimes corresponding to successive dynamical regimes: a dispersed phase before the food is introduced, followed by a food-exchange phase in which clusters form.

## [03128] What does Multivector Fields Theory have to offer?

**Format :** Talk at Waseda University

**Author(s) :** Michał Lipiński (Polish Academy of Sciences)

**Abstract :** The theory of Multivector Fields (MVF) is a generalization of Forman vector fields. It has been continuously developed since 2017. MVF theory is equipped with a number of fundamental dynamical concepts and matures into a useful combinatorial model for classical vector fields. In the talk I will present the general idea of the MVF theory, its suitability for the analysis in the spirit of topological data analysis, and its usefulness in understanding continuous dynamical systems.

## [03410] A Persistence-like Algorithm for Computing Connection Matrices Efficiently

**Format :** Talk at Waseda University

**Author(s) :** Tamal Krishna Dey (Purdue University)

**Abstract :** Connection matrices are a generalization of Morse boundary operators from the classical Morse theory for gradient vector fields. Developing an efficient computational framework for connection matrices is particularly important in the context of a rapidly growing data science that requires new mathematical tools for discrete data. Toward this goal, the classical theory for connection matrices has been adapted to combinatorial frameworks that facilitate computation. We develop an efficient persistence-like algorithm to compute a connection matrix from a given combinatorial (multi) vector field on a simplicial complex. This algorithm requires a single-pass, improving upon a known algorithm that runs an implicit recursion executing two-passes at each level. Overall, the new algorithm is more

part\_1

simple, direct, and efficient than the state-of-the-art. Because of the algorithm's similarity to the persistence algorithm, one may take advantage of various software optimizations from topological data analysis.

This is a joint work with Michal Lipinski, Marian Mrozek, and Ryan Slechta

00595 (2/3) : 5C @G802 [Chair: Thomas Wanner]

## [04935] A combinatorial/homological framework for continuous nonlinear dynamics

**Format :** Talk at Waseda University

**Author(s) :** Konstantin Mischaikow (Rutgers University)

**Abstract :** Computational science and data-driven science suggests the importance of having finite models of dynamics. This raises three questions: 1. How to go from data to appropriate combinatorial models of dynamics. 2. What computations should be performed on these combinatorial models. 3. How to translate the output from the combinatorial models to structures associated with continuous systems. In this talk we will discuss our attempts to provide a coherent approach to addressing these questions.

## [04988] Computing the Global Dynamics of Parameterized Systems of ODEs

**Format :** Talk at Waseda University

**Author(s) :** Marcio Gameiro (Rutgers University)

**Abstract :** We present a combinatorial topological method to compute the dynamics of a parameterized family of ODEs. A discretization of the state space of the systems is used to construct a combinatorial representation from which recurrent versus non-recurrent dynamics are extracted. Algebraic topology is then used to validate and characterize the dynamics of the system. We will discuss the combinatorial description and the algebraic topological computations and will present applications to systems of ODEs arising from gene regulatory networks.

## [04981] Combinatorics and Topology for Understanding Global Dynamics in Multi-Scale Systems.

**Format :** Talk at Waseda University

**Author(s) :** Ewerton Rocha Vieira (Rutgers University)

**Abstract :** This talk introduces a new approach to analyzing time-varying systems with multi-scale dynamics, which can be challenging due to poorly measured parameters and numerous variables. Traditionally, these systems are modeled using ordinary differential equations (ODE), but this approach can be difficult to apply directly. The proposed approach is based on combinatorics and algebraic topology, and focuses on describing global dynamics in terms of annotated graphs (Morse graphs) and Conley complexes. The method is based on piecewise linear models and offers a more robust, scalable, and computable description of dynamics than classical ODE analysis, with formal mathematical guarantees that extend to a class of ODE with steep sigmoidal nonlinearities. This approach is particularly useful for modeling complex systems, such as biological systems.

## [04843] On the identification of cycling motion using topological tools

**Format :** Talk at Waseda University

**Author(s) :** Ulrich Bauer (Technical University of Munich)David Hien (Technical University of Munich)Oliver Junge (Technical University of Munich)Konstantin Mischaikow (Rutgers University)

**Abstract :** Nonlinear dynamical systems often exhibit complicated recurrent behaviour. We propose to decompose recurrent sets into elementary oscillations and the connections between them. To this end, we use topological tools that are flexible enough to be computed from data while still providing a comprehensive description of the oscillations. We demonstrate this through several examples. In particular, we identify and analyze 6 oscillations in a 4d hyperchaotic attractor.

00595 (3/3) : 5D @G802 [Chair: Marian Mrozek]

## [03335] Morse-Smale quadrangulations and persistence of vector fields

**Format :** Talk at Waseda University

**Author(s) :** Claudia Landi (Università di Modena e Reggio Emilia)Clemens Luc Bannwart (Università di Modena e Reggio Emilia)

**Abstract :** The goal of this talk is to introduce a persistence barcode for discrete gradient vector fields defined on a combinatorial 2-manifold. The main ingredient is a decomposition of the manifold into quadrangle regions with vertices ordinally given by sinks, saddles, sources, and saddles. We will consider a bottleneck distance and an interleaving distance for such barcodes and we will present results about their stability.

part\_1

## [04607] On the dynamics of the combinatorial model of the real line

**Format :** Online Talk on Zoom

**Author(s) :** Pedro J. Chocano (Rey Juan Carlos University)

**Abstract :** In this talk, we describe the dynamics that appear when we consider a discrete dynamical system defined on the combinatorial model of the real line. Particularly, we show that there are no periodic points of period greater than or equal to 3, which contrasts with the classical setting (Sharkovski theorem). This fact motivates us to introduce multivalued maps to get richer dynamics than the ones obtained from single valued maps. To conclude we provide some examples.

## [04886] Topological Inference of the Conley Index

**Format :** Online Talk on Zoom

**Author(s) :** Vidit Nanda (University of Oxford)Ka Man Yim (University of Oxford)

**Abstract :** The Conley index of an isolated invariant set is a fundamental object in the study of dynamical systems. Here we consider smooth functions on closed submanifolds of Euclidean space and describe a framework for inferring the Conley index of any compact, connected isolated critical set of such a function with high confidence from a sufficiently large finite point sample. The main construction of this paper is a specific index pair which is local to the critical set in question. We establish that these index pairs have positive reach and hence admit a sampling theory for robust homology inference. This allows us to estimate the Conley index, and as a direct consequence, we are also able to estimate the Morse index of any critical point of a Morse function using finitely many local evaluations.

## [05010] Analysis of solids regarded as compositions of discrete entities

**Format :** Online Talk on Zoom

**Author(s) :** Andrey Jivkov (The University of Manchester)

**Abstract :** In contrast with the idealisation of materials as continua, their internal structures are regarded here as polyhedral complexes. One approach to formulate conservation laws of scalar (mass, energy, charge) and vector (linear and angular momentum) quantities on such complexes is presented. It uses combinatorial differential forms, representing physical quantities, and operations with such forms (exterior derivatives, exterior products, and codifferentials), describing processes and conservations. The derived conservation laws are background independent.

# [00598] Hyperplane arrangements and enumerative problems

**Session Time & Room :** 2C (Aug.22, 13:20-15:00) @A617

**Type :** Proposal of Minisymposium

**Abstract :** Hyperplane arrangements appear in many areas of mathematics, including topology, combinatorics, algebraic geometry. One of the important aspects is that hyperplane arrangements have several discrete structures e.g., poset of intersections, chambers, lattice points. Enumerations of these objects play crucial roles in many problems, e.g., enumerative problems, coding theory. In this minisymposium, we focus on enumerative aspects of these objects.

**Organizer(s) :** Masahiko Yoshinaga, Norihiro Nakashima

**Classification :** 52C35, 05C31

**Minisymposium Program :**

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00598 (1/1) : 2C @A617 [Chair: Takuro Abe]

## [01887] Coboundary polynomial and related polynomial invariants

**Format :** Talk at Waseda University

**Author(s) :** Norihiro Nakashima (Nagoya Institute of Technology)

**Abstract :** The coboundary polynomial is a polynomial computed by all characteristic polynomials for restriction arrangements to all flats in the intersection poset. It is known that the coboundary polynomial is essentially the same as the weight enumerator and Tutte polynomial. In this talk, we introduce some known results about these relationship and future issues.

## [01889] Generalizations of Tutte-Grothendieck polynomials

**Format :** Talk at Waseda University

**Author(s) :** Tsuyoshi Miezaki (Waseda University) HIMADRI SHEKHAR CHAKRABORTY (Shahjalal University of Science and Technology) CHONG ZHENG (Waseda University)

**Abstract :** A Tutte-Grothendieck polynomial is a graph invariant that satisfies a generalized deletion-contraction formula. In this talk, we introduce the notion of weighted Tutte-Grothendieck polynomial and weighted Tutte-Grothendieck invariant for matroid and discuss some of its properties. Moreover, we show that the weighted Tutte-Grothendieck invariant is stronger than the Tutte-Grothendieck invariant. This is joint work with Himadri Chakraborty (SUST) and Chong Zheng (Waseda University).

## [01791] Characteristic quasi-polynomials of arrangements over algebraic integers

**Format :** Talk at Waseda University

**Author(s) :** Shuhei Tsujie (Hokkaido University of Education)

**Abstract :** Kamiya, Takemura, and Terao initiated the theory of the characteristic quasi-polynomial of an integral arrangement, which is a function counting the elements in the complement of the arrangement modulo positive integers.

In this talk, we will discuss arrangements over the rings of integers of algebraic number fields.

## [01780] Counting the regions of hyperplane arrangements related to Coxeter arrangements.

**Format :** Online Talk on Zoom

**Author(s) :** Yasuhide Numata (Hokkaido University)

**Abstract :** We consider the Shi and Ish arrangement of type  $B_n$ . Both are hyperplane arrangements in the real vector space of dimension  $n$  containing the Coxeter arrangement of type  $B_n$ . We discuss combinatorial objects which parametrize the regions, i.e. connected components of complement of the arrangement, of these arrangement.

# [00603] Mean field stochastic control problems and related topics

**Session Time & Room :** 1C (Aug.21, 13:20-15:00) @E502

**Type :** Proposal of Minisymposium

**Abstract :** Mean-field (or, McKean-Vlasov) SDEs have been studied for a long time and have found lots of applications in different domains. Recently, with their pioneering seminal papers (2006-2007) on mean-field games and their applications in economics, finance and game theory, Lasry and Lions have given new impulses to this research topic, opened the way to new applications and attracted lots of researchers to this topic. One of these applications is the study of mean-field stochastic optimal control problems. In our symposium we will study the viability property for controlled mean-field flows, the mass-conserving SPDE coming from spatial mean-field term, etc.

**Organizer(s) :** Juan Li

**Classification :** 60H10, 60K35, 93E03

**Minisymposium Program :**

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00603 (1/1) : 1C @E502

## [01320] Stochastic maximum principle for weighted mean-field system

**Format :** Talk at Waseda University

**Author(s) :** Jie Xiong (Southern University of Science and Technology)

**Abstract :** We study the optimal control problem for a weighted mean-field system. A new feature of the control problem is that the coefficients depend on the state process as well as its weighted measure and the control variable. By applying variational technique, we establish a stochastic maximum principle. Also, we establish a sufficient condition of optimality. As an application, we investigate the optimal premium policy of an insurance firm for asset-liability management problem. This talk is based on a joint paper with Yanyan Tang.

## [00653] The mass-conserving stochastic partial differential equation coming from spatial mean-field term

**Format :** Talk at Waseda University

**Author(s) :** Qi Zhang (Fudan University)

**Abstract :** In this talk, I will introduce our study about the mass-conserving stochastic partial differential equation. It is a kind of equation with spatial mean-field term such that its solution satisfies a mass-conservative property. We prove the existence and uniqueness of solution, and then construct a stationary solution by the nonlinear Feynman-Kac formula under Lipschitz assumption. Moreover, the existence of solution in the non-Lipschitz case is considered.

## [01321] A quadratic mean-field BSDE with its applications

**Format :** Talk at Waseda University

**Author(s) :** Huilin Zhang (Shandong University)

**Abstract :** In this talk I will introduce the well-posedness of a quadratic mean-field BSDE.

Moreover we show its several applications, in particular in the utility theory.

## [01324] Mean field stochastic control under sublinear expectation

**Format :** Talk at Waseda University

**Author(s) :** Juan Li (Shandong University)

**Abstract :** In this talk we study Pontryagin's stochastic maximum principle for a mean-field optimal control problem under Peng's  $G$ -expectation. The dynamics of the controlled state process is given by a SDE driven by a  $G$ -Brownian motion, whose coefficients depend not only on the control, the controlled state process but also on its law under the  $G$ -expectation. Also the associated cost functional is of mean-field type. We give a necessary optimality condition for control processes, and also a sufficient one. The main difficulty which we have to overcome in our work consists in the differentiation of the  $G$ -expectation of parameterized random variables.

Based on joint work with Rainer Buckdahn (UBO, France), Bowen He (SDU, China).

# [00604] Frontiers of Collaboration with Industry: Towards International Mathematical Commons

**Session Time & Room :**

00604 (1/2) : 3C (Aug.23, 13:20-15:00) @G301

00604 (2/2) : 3D (Aug.23, 15:30-17:10) @G301

**Type :** Proposal of Industrial Minisymposium

**Abstract :** This mini-symposium introduces the forefront of various organizational initiatives aimed at mathematical research and educational institutions around the world using the power of mathematics for solving industrial problems, including activities to provide a basic environment and to promote the building of relationships with industry. By sharing not only the outputs but also various issues and solutions conducted through these activities with participants, we expect to contribute to the formation of an international platform, a mathematical common, where mathematicians, together with industry, can overcome the myriad of difficulties our society must confront.

**Organizer(s) :** Kenji Kajiwara, Takashi Sakajo, Hiroshi Suito

**Classification :** 00A05, 00A06, 00A69, 00A71, 00A72

**Minisymposium Program :**

00604 (1/2) : 3C @G301 [Chair: Takashi Sakajo]

## [01978] The UniSA Mathematics Clinic: How to build a work-integrated-learning ecosystem

**Format :** Talk at Waseda University

**Author(s) :** Lesley Ann Ward (University of South Australia)

**Abstract :** The University of South Australia Mathematics Clinic runs yearlong authentic industry-sponsored research projects for small teams of final-year undergraduate mathematics students. I will outline how to build the necessary commitment and structure for such a programme, touching on curriculum; articulation with other mathematics courses; part\_1

coaching students in professional skills and leadership roles; pitching and recruitment of industry sponsors; engaging students and academic staff; intellectual property, confidentiality, and contracts; and scoping and development of suitable projects.

## **[02932] Industrial Student Research Programs and Industry Connections at IPAM**

**Format :** Talk at Waseda University

**Author(s) :** Christian Ratsch (UCLA)

**Abstract :** The goal of the Institute for Pure and Applied Mathematics (IPAM) is to foster the interaction of mathematics with a broad range of science and technology. In this talk I will review and discuss some of the IPAM activities that are used to fulfill this goal. I will discuss the Research in Industrial Projects for Students (RIPS) program, where undergraduate students work in teams on projects that have been sponsored by an industrial partner.

## **[01963] Development of Mathematics for Industry in Japan: New Research Area, Education and Platform**

**Format :** Talk at Waseda University

**Author(s) :** Kenji Kajiwara (Institute of Mathematics for Industry, Kyushu University)

**Abstract :** In this talk, we exhibit activities of "Mathematics for Industry" (MfI) in Japan, initiated by the Institute of Mathematics for Industry( IMI), Kyushu University founded in 2011. MfI intends to develop a new research area of mathematics formed by responding to the needs of industries associated with various relevant activities such as education and network/platform formed by mathematicians and mathematical institutes. We present various challenges to realizing the idea of MfI in Japan.

## **[01984] APCMfI and International Mathematical Commons for Asia Pacific region**

**Format :** Online Talk on Zoom

**Author(s) :** Zainal Abdul Aziz (Universiti Teknologi Malaysia)

**Abstract :** In order to facilitate Mathematics for Industry-MfI within the platform of International Mathematical Commons for Asia Pacific region i.e., encompassing academia, industrial, government and communal sectors; then APCMfI have to implement more effective mechanisms. These include fostering Asia Pacific Study Groups with Industry, proposing Centres of MfI-based in Universities, establishing Asia Pacific Networks, promoting National Networks, supporting Conferences and Workshops on Industrial Problems, Student Programmes and Modelling Camps, Internships and Industry/Academia Exchanges and Consultancy.

00604 (2/2) : 3D @G301 [Chair: Kenji Kajiwara]

## **[01944] European Consortium for Mathematics in Industry - research and education**

**Format :** Talk at Waseda University

**Author(s) :** Alessandra Micheletti (Università degli Studi di Milano)

**Abstract :** The European Consortium for Mathematics in Industry (ECMI) is a consortium of academic institutions and industrial companies that acts co-operatively to promote and support the use of mathematical modelling, simulation, and optimization in any activity of social or economic importance. ECMI is devoted to research motivated by industrial problems and education of Industrial Mathematicians to meet the growing demand for such experts. In this talk we will present an overview of ECMI activities in research, education and international cooperation.

## **[01965] EU-MATHS-IN OpenDesk. Un infrastructure to boost industry's competitiveness.**

**Format :** Online Talk on Zoom

**Author(s) :** Manuel Cruz (EU-MATHS-IN OpenDesk; LEMA-ISEP | Instituto Superior de Engenharia do Porto)Véronique Maume-Deschamps (EU-MATHS-IN OpenDesk; Université Claude Bernard Lyon 1 | Institut Camille Jordan)Peregrina Quintela Estévez (EU-MATHS-IN OpenDesk; CITMAga)Alexander Scherrer (EU-MATHS-IN OpenDesk; Fraunhofer Institute for Industrial Mathematics ITWM)Antonino Sgalambro (EU-MATHS-IN OpenDesk; Sheffield University Management School; National Research Centre of Italy)Janusz Sztabinski (EU-MATHS-IN OpenDesk; Wrocław University of Science and Technology)

**Abstract :** The EU-MATHS-IN OpenDesk is a one-stop-shop aimed to make companies more competitive through mathematical technologies (MSODE). It facilitates the access to the best European technology transfer centres and

coordinates the looking for the most appropriate partners to solve the current challenges.  
 In this talk, the main points of interest of the OpenDesk will be introduced as well as its main services and procedures.

## [02986] mathematics in the society: rethinking its role, one graduate student at a time.

**Format :** Online Talk on Zoom

**Author(s) :** yuliy baryshnikov (UIUC)

**Abstract :** Each year, a wave of new PhD in mathematics graduate. Statistically just about half of them will find a position in academia. How are we preparing the rest to the increasingly important role the mathematicians play in the modern society?

In this talk I will present some observations and experiences from perspectives of both academic and industrial research departments.

## [05594] A Knowledge Exchange Hub for the Mathematical Sciences

**Format :** Online Talk on Zoom

**Author(s) :** Ulrike Tillmann (Isaac Newton Institute)

**Abstract :** An influential 2018 review of knowledge exchange (KE) in the mathematical sciences in the UK called for an improved infrastructure at national level. Five years later, we report on the journey towards a KE-Hub, its vision and ambitions. An important part of the journey was the award winning Virtual Forum for KE in the Mathematical Sciences (V-KEMS) set-up during the pandemic.

## [00605] Recent advances in theory and application of quantum computing technology

**Session Time & Room :**

00605 (1/3) : 4C (Aug.24, 13:20-15:00) @D405

00605 (2/3) : 4D (Aug.24, 15:30-17:10) @D405

00605 (3/3) : 4E (Aug.24, 17:40-19:20) @D405

**Type :** Proposal of Minisymposium

**Abstract :** There are great expectations for quantum computing, and various efforts are being made to develop its hardware and software.

However, its scale is currently inferior, and the discrepancy is enormous compared to the high-performance computing (HPC) field.

Quantum annealing also still has many challenges in its application to practical problems.

Basic research on quantum computers is expected to develop further in the future.

In this minisymposium, we present research on quantum computing technology, especially the theory and practice of quantum annealing.

The implementations of quantum annealing will be covered both quantum annealers and quantum-inspired annealers.

**Organizer(s) :** Tomohiro Suzuki

**Classification :** 81-10, 81P68, Quantim annealing

**Minisymposium Program :**

00605 (1/3) : 4C @D405 [Chair: Kazuhiko Komatsu]

## [03620] QUBO encoding of inequality constraints in Quantum Minimum Fill-in algorithm

**Format :** Talk at Waseda University

**Author(s) :** Tomoko Komiyama (University of Yamanashi)Tomohiro Suzuki (University of Yamanashi)

**Abstract :** Expressing constraints with complex conditions in terms of inequalities in solving optimization problems is common. When solving problems with quantum annealing, inequality constraints must be transformed into an unconstrained quadratic form that does not contain inequalities. There are various methods for this transformation,

which vary in the number of auxiliary variables to be added and the total number of solutions that will be optimal. We compare these transformation methods and discuss which is suitable for quantum annealing.

## [02807] Approximate block diagonalization of symmetric matrices using a quantum annealing

**Format :** Talk at Waseda University

**Author(s) :** Koshi Teramoto (The University of Electro-Communications)Masaki Kugaya (The University of Electro-Communications)Shuhei Kudo (The University of Electro-Communications)Yusaku Yamamoto (The University of Electro-Communications)

**Abstract :** Approximate block diagonalization is an efficient preprocessing technique for accelerating the block Jacobi method to solve the symmetric eigenvalue problem.

The aim of this study is to speed up this process using quantum annealing.

To achieve this, we formulated it as a combinatorial optimization problem and expressed it in Quadratic Unconstrained Binary Optimization (QUBO) that can be dealt with by D-Wave's quantum annealing system.

Numerical experiments on small matrices using D-Wave Advantage show that optimal approximate block diagonalization that minimizes the off-diagonal norm can be obtained with high probability.

## [03304] Performance evaluation of quantum-inspired machine and quantum simulator

**Format :** Talk at Waseda University

**Author(s) :** Makoto Morishita (Nagoya University)Takahiro Katagiri (Nagoya University)Satoshi Ohshima (Kyusyu University)Tetsuya Hoshino (Nagoya University)Toru Nagai (Nagoya University)

**Abstract :** The purpose of this research is to construct a heterogeneous environment in which next-generation computers that quantum computers are equipped as an accelerator specialized for specific calculations (e.g., solving QUBO).

The performance of annealing-base and gate-base by benchmarks is evaluated as a preliminary result. In particular, we evaluated the performance of solving QUBO by the annealing-base such as digital annealers, and by the gate-base of quantum circuits implementing QAOA.

Hyperparameters such as coefficients of constraint terms appearing in the QUBO formula, and the number of unitary gates in QAOA, are tuned by utilizing Optuna in our experiment.

## [03892] Use of digital annealer for HPC applications

**Format :** Talk at Waseda University

**Author(s) :** Masatoshi kawai (Nagoya University)

**Abstract :** In some high-performance applications, combinatorial optimization problems (COPs) are solved in unique methods. However, solving these COPs with more constraint conditions and complex evaluation functions may improve the performance of the applications. In this study, we discuss the performance improvement obtained by using Digital Annealing to solve the complex COPs derived from lattice H-matrices with dynamic load balancing and the parallelized incomplete Cholesky conjugate gradient method using a multi-coloring technique.

00605 (2/3) : 4D @D405 [Chair: Tomohiro Suzuki]

## [04414] Performance Evaluation of Ising Machines using Constraint Combinatorial Optimization Problems

**Format :** Talk at Waseda University

**Author(s) :** Kazuhiko Komatsu (Tohoku University)Makoto Onoda (Tohoku University)Masahito Kumagai (Tohoku University)Hiroaki Kobayashi (Tohoku University)

**Abstract :** Ising machines have been developed rapidly by various implementations. However, the characteristics of Ising machines have not been clarified yet because a unified evaluation method and commonly used benchmark program for Ising machines have not been established.

This research evaluates various Ising machines using constraint combinatorial optimization problems. Through the evaluation, the characteristics of Ising machines are clarified.

## [04218] Nonnegative binary matrix factorization by continuous relaxation and reverse annealing

**Format :** Talk at Waseda University

**Author(s) :** Renichiro Haba (Tohoku University)Masayuki Ohzeki (Tohoku University)Kazuyuki Tanaka (Tohoku University)

**Abstract :** In this talk, we introduce a reverse annealing framework with relaxation strategies for nonnegative/binary matrix factorization, a feature extraction technique. Reverse annealing is one of the quantum annealing techniques and its specific usage has not been well explored. Experimental results reveal performance comparable to exact optimization methods, indicating the potential for expanding the applicability of reverse annealing.

## [03976] Kernel learning by quantum annealer

**Format :** Talk at Waseda University

**Author(s) :** Yasushi Hasegawa (Tohoku University)Hiroki Oshiyama (Tohoku University)Masayuki Ohzeki (Tohoku University)

**Abstract :** Kernel methods are powerful in machine learning. It is known that shift-invariant kernels can be represented by Fourier transformation of a probability distribution of frequencies. Recently the method called Implicit Kernel Learning is proposed, which learns the probability distribution according to the given data by generative model.

We developed a new method that uses quantum annealing as a sampler to train Boltzmann machines for the probability distribution. We demonstrate our method by using D-Wave quantum annealer.

00605 (3/3) : 4E @D405 [Chair: Takahiro Katagiri]

## [03609] mpiQulacs: A Distributed Quantum Computer Simulator for A64FX-based Cluster Systems

**Format :** Talk at Waseda University

**Author(s) :** Masafumi Yamazaki (Fujitsu LTD.)Satoshi Immura (Fujitsu LTD.)Takumi Honda (Fujitsu LTD.)Akihiko Kasagi (Fujitsu LTD.)Akihiro Tabuchi (Fujitsu LTD.)Hiroshi Nakao (Fujitsu LTD.)Naoto Fukumoto (Fujitsu LTD.)Kohta Nakashima (Fujitsu LTD.)

**Abstract :** Quantum computer simulators running on classical computers are essential for understanding real quantum states and developing emerging quantum applications. In particular, state-vector simulators, which store the complete state vector in memory can be used to analyze the behavior of all types of quantum applications.

Here, we briefly introduce a distributed state-vector simulator and describe its distributed implementation and optimization. Finally, we present the scaling performance of the large-scale simulation using an A64FX-based cluster system.

## [04257] Examples of application of CMOS annealing

**Format :** Talk at Waseda University

**Author(s) :** Akiko Masaki (Hitachi, Ltd.)Kaho Takahashi (Hitachi, Ltd.)Kazuo Ono (Hitachi, Ltd.)Taro Aratani (National Institute of Maritime, Port and Aviation Technology)Takahiro Majima (National Institute of Maritime, Port and Aviation Technology)

**Abstract :** Hitachi has developed CMOS annealing technology as a next-generation computing technology that can solve large-scale, complex optimization problems at high speed.

In this talk, we will introduce some examples of practical applications of CMOS annealing technology. In particular, we will present examples of applications that are proving effective in the field of public infrastructure, where there are large-scale problems that cannot be solved by conventional computing technologies.

## [04116] Outline and present development status of CMOS annealing

**Format :** Talk at Waseda University

**Author(s) :** Masanao Yamaoka (Hitachi, Ltd.)

**Abstract :** Today, optimization processing is important for various fields. The CMOS annealing technology, which is a new-paradigm computing technology inspired by quantum computers, was developed to accelerate the optimization processing for the new value creation. By utilizing semiconductor technology, CMOS annealing can achieve large-scale integration and can be easily implemented for the practical usage. In this talk, the outline of CMOS annealing will be introduced with some examples of actual applications as a present development status.

# [00607] Analysis and computation of interface evolution equation and related topics

**Session Time & Room :** 5C (Aug.25, 13:20-15:00) @F411

**Type :** Proposal of Minisymposium

**Abstract :** Analyzing and computational methods for interfacial motion including some singularities or topological changes has been continued to develop and applied to various fields. Recently, these methods are extended to the problems with strong singularity and constraint, nonlocal evolution law, or coupling system and other phenomena. In these developments, there has been high demand for fast and accurate computing, and rigorous mathematical analysis of parametric or non-parametric interface motion. This minisymposium will feature the recent developments on modelling, computation and analysis for interface evolution equation involving the above motivation and related topics.

**Organizer(s) :** Takeshi Ohtsuka, Yoshihito Kohsaka

**Classification :** 53E10, 53E40, 65M22, 35K65, 35K67

**Minisymposium Program :**

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00607 (1/1) : 5C @F411 [Chair: Yoshihito Kohsaka]

## [03814] A minimizing movement approach to surface constrained interfacial motions

**Format :** Talk at Waseda University

**Author(s) :** Elliott Ginder (Meiji University)

**Abstract :** By extending the applicability of minimizing movements to the surface PDE setting, we will develop threshold dynamics for surface-constrained interfacial motions. In particular, we will show how our approach enables one to approximate multiphase, volume-preserving, curvature flows on surfaces via generalized MBO and HMBO algorithms.

## [02801] Geometric Sobolev gradient flows on spaces of curves

**Format :** Talk at Waseda University

**Author(s) :** Philip Schrader (Murdoch University)

**Abstract :** The curve-shortening flow, which deforms a closed planar curve by moving its points perpendicular to the curve with velocity proportional to curvature, was proposed by Mullins as a model for the motion of grain boundaries in the process of annealing. It can be characterised as the gradient descent of the length functional on curves, when the gradient is taken with respect to a parametrisation invariant  $L^2$  inner product. In this talk I will describe some of the gradient flows which result when taking instead the gradient with respect to some Sobolev parametrisation invariant inner products. I will discuss the different kinds of asymptotic behaviour that are possible and also the numerical advantages of  $H^1$  products.

## [03938] A Simple Algorithm for the Monge-Ampere Equation on a Sphere

**Format :** Talk at Waseda University

**Author(s) :** Richard Tsai (The University of Texas at Austin)Axel Turnquist (University of Texas at Austin)

**Abstract :** In this talk, we present a novel approach for solving the Monge-Ampere (MA) equation defined on a sphere. Specifically, we extend the MA equation on a sphere to a narrowband around the sphere by formulating an equivalent optimal transport problem. We demonstrate that the extended MA equation can be solved using existing algorithms developed for the MA equation on Euclidean space, making the resulting algorithm simple and easy to implement. Our approach provides a useful tool for solving problems that involve the MA equation defined on or near a sphere, which has a wide range of applications in fields such as computer graphics, image processing, and fluid dynamics.

## [02029] Waiting time effects for the wearing process of a non-convex stone

**Format :** Talk at Waseda University

**Author(s) :** Nao Hamamuki (Hokkaido University)Ryosuke Takahashi (Hokkaido University)

**Abstract :** We investigate evolution of a non-convex stone by the wearing process. Following the formulation introduced by Ishii and Mikami 2001, 2004, we study the unique viscosity solution of a nonlocal Gauss curvature flow equation describing the wearing process and prove that waiting time effects occur on an appropriate subset in a cavity of the stone, that is, any point on the set does not move at all for some positive time.

# [00608] Limit behavior and asymptotic properties in fluid mechanics

## Session Time & Room :

00608 (1/3) : 3E (Aug.23, 17:40-19:20) @G703

00608 (2/3) : 4C (Aug.24, 13:20-15:00) @G703

00608 (3/3) : 4D (Aug.24, 15:30-17:10) @G703

## Type : Proposal of Minisymposium

**Abstract :** The mathematical analysis of problems from fluid mechanics under the passage to certain limits can lead to new insights into the underlying physics and can help to improve numerical implementations. This minisymposium brings together scientists studying such kinds of asymptotic behaviors in different settings. The speakers present their research on homogenization problems and singular limits for fluid models, as well as on long-time and far-field behavior of fluid flows. Bringing together scientists working on these very different kinds of limit problems might create synergies between their approaches that usually differ significantly.

**Organizer(s) :** Thomas Eiter, Florian Oschmann

**Classification :** 35Q35, 76M45, 76M50

## Minisymposium Program :

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00608 (1/3) : 3E @G703 [Chair: Thomas Eiter]

## [01787] Homogenization of nonstationary incompressible viscous non-Newtonian flows

### Format : Talk at Waseda University

**Author(s) :** Yong Lu (NANJING UNIVERSITY)Zhengmao Qian (NANJING UNIVERSITY)

**Abstract :** We consider the homogenization of the nonstationary incompressible viscous non-Newtonian fluid flows in a domain perforated with a large number of tiny holes, where the size of the holes is proportional to the mutual distance of the holes, and the stress tensor satisfies the Carreau-Yasuda law. Darcy's law is derived in the limit as the size of holes goes to zero and the number of holes goes to infinity simultaneously.

## [05572] Homogenization of compressible Navier-Stokes in critically perforated domains in Limit behavior and asymptotic properties in fluid mechanics

### Format : Talk at Waseda University

**Author(s) :** Peter Bella (TU Dortmund)Friederike Lemming (TU Dortmund)Roberta Marziani (TU Dortmund)Florian Oschmann (Czech Academy of Sciences)

**Abstract :** We consider homogenization of the time-dependent compressible Navier-Stokes equations in the low Mach number regime in critically periodically perforated domains. In analogy to a classical result of Allaire (ARMA 90) for the incompressible fluids, we obtain in the limit the incompressible Navier-Stokes system with an additional Brinkman friction form.

## [05422] Existence of weak solutions and hard-congestion limit in the dissipative Aw-Rascle system

### Format : Online Talk on Zoom

**Author(s) :** Ewelina Zatorska (Imperial College London)Nilasis Chaudhuri (Imperial College London)

**Abstract :** In this talk I am going to present the dissipative Aw-Rascle model of evolution of congestions. I will first explain its connection with other models in fluid mechanics (compressible Euler and Navier-Stokes) and present our progress on the existence theory. In the second part of my talk I will focus on discussing a singular limit passage leading to the so-called "hard-congestion" system.

## [01575] $\Gamma$ -convergence of nearly incompressible fluids

### Format : Talk at Waseda University

**Author(s) :** Peter Bella (TU Dortmund)Eduard Feireisl (Czech Academy of Sciences)Florian Oschmann (Czech Academy of Sciences)

**Abstract :** We consider the time-dependent compressible Navier-Stokes equations in the low Mach number regime in a family of domains  $\Omega_\varepsilon \subset \mathbb{R}^d$  converging in the sense of Mosco to a domain  $\Omega \subset \mathbb{R}^d$ ,  $d \in \{2, 3\}$ . We show the limit is the part\_1

incompressible Navier–Stokes system in  $\Omega$ . This is joint work with Peter Bella (TU Dortmund) and Eduard Feireisl (CAS).

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00608 (2/3) : 4C @G703 [Chair: Thomas Eiter]

## [04842] Invariant manifolds for the thin film equation

**Format :** Talk at Waseda University

**Author(s) :** Christian Seis (University of Munster)Dominik Winkler (University of Munster)

**Abstract :** The large-time behavior of solutions to the thin film equation with linear mobility in the complete wetting regime on  $R^N$  is examined: We investigate the higher order asymptotics of solutions converging towards self-similar Smyth–Hill solutions under certain symmetry assumptions on the initial data. The analysis is based on a construction of finite-dimensional invariant manifolds that solutions approximate to an arbitrarily prescribed order.

## [03881] The Navier-Stokes flow in the exterior Lipschitz domain

**Format :** Talk at Waseda University

**Author(s) :** Keiichi Watanabe (Suwa University of Science)

**Abstract :** Consider the three-dimensional Navier-Stokes equations in an exterior Lipschitz domain  $\Omega$ . In this talk, we show the unique existence of a global strong solution  $u$  to the Navier-Stokes equations and investigate the large time behavior of the solution  $u$ . Although the boundary is not smooth, we show that the large time behavior of the Navier-Stokes flow is completely recovered in the exterior Lipschitz domain  $\Omega$  along exactly the same argument as usual.

## [04533] Anisotropically spatial-temporal behavior of the Navier-Stokes flow past an obstacle

**Format :** Talk at Waseda University

**Author(s) :** Tomoki Takahashi (Tokyo Institute of Technology)

**Abstract :** We consider the spatial-temporal behavior of the Navier-Stokes flow past a three dimensional rigid body and deduce

the temporal decay rate with the spatial weight caused by translation. The key tool is the  $L^q$ - $L^r$  estimate of the Oseen semigroup in exterior domains and we develop the weighted  $L^q$  theory of the Oseen semigroup. New results on the Stokes semigroup in isotropic  $L^q$  spaces are also discussed.

## [01603] Stokes and Oseen fundamental solutions: asymptotic properties of fluid flows and applications in computational fluid dynamics

**Format :** Talk at Waseda University

**Author(s) :** Ana Leonor Silvestre (Instituto Superior Técnico, Universidade de Lisboa)

**Abstract :** Starting from the Stokes and Oseen steady and unsteady fundamental solutions, we discuss asymptotic properties of fluid flow around a translating and rotating rigid body. This part of the talk includes joint work with Toshiaki Hishida, from Nagoya University, Japan, and Takéo Takahashi, from INRIA Nancy - Grand Est, France. In the second part of the talk, based on joint work with Carlos Alves, Rodrigo Serrão, from Instituto Superior Técnico, Portugal, and Svilen Valtchev, from Instituto Politécnico de Leiria, Portugal, we present a numerical study of the Method of Fundamental Solutions for Stokes and Oseen boundary value problems. The accuracy of the method is illustrated through a series of numerical tests, which include a comparison between analytic and numerical solutions and the application of the method to classical benchmark problems.

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00608 (3/3) : 4D @G703 [Chair: Florian Oschmann]

## [04660] Multiscale analysis - from compressible to incompressible system

**Format :** Talk at Waseda University

**Author(s) :** Aneta Wróblewska-Kamińska (Institute of Mathematics, Polish Academy of Sciences)

**Abstract :** We will show asymptotic analysis for hydrodynamic systems as a tool in the situation when certain parameters

vanish or become infinite. We will concentrate on rigorous mathematical analysis of low Mach number limits with so called ill-prepared data. I will present some results which concerns passage from compressible to incompressible models including Navier-Stokes-Fourier system on varying domains, a multi-scale problem for viscous heat-conducting fluids in fast rotation and FENE model for dilute polymeric fluids.

## [04114] Mixing and enhanced dissipation for fluid suspensions

**Format :** Talk at Waseda University

**Author(s) :** David Gerard-Varet (Universite Paris Cite et IMJ-PRG)

**Abstract :** We consider a model introduced by D. Saintillan and M. Shelley to describe active suspensions of elongated particles. This model couples a Stokes equation for the fluid substrate and a transport equation for the density distribution of

particles in space and orientation. We investigate mixing properties of this model (damping and enhanced dissipation). The main new feature of the analysis is that the usual velocity variable of the euclidean space is replaced by an orientation variable on the sphere, which is responsible for strong qualitative changes and new mathematical difficulties. This is joint work with M. Coti Zelati and H. Dietert.

## [05036] Resolvent estimate for the Stokes equations in the Besov spaces

**Format :** Talk at Waseda University

**Author(s) :** Jou chun Kuo (Graduate School of Fundamental Science and Engineering, Waseda University)

**Abstract :** This talk is devoted to proving the resolvent estimates of the linearized system of the compressible Navier-Stokes equations with homogeneous boundary conditions in the half-space. We construct the solution in  $B_{q,1}^s$  for  $s \in$

## [05215] Conditions for energy balance in 2D incompressible ideal fluid flow

**Format :** Online Talk on Zoom

**Author(s) :** Milton da Costa Lopes Filho (Universidade Federal do Rio de Janeiro) Samuel Lanthaler (California Institute of Technology) Fabian Jin (ETH-Zurich) Helena Judith Nussenzveig Lopes (Universidade Federal do Rio de Janeiro)

**Abstract :** In this talk I will discuss necessary and sufficient conditions on the regularity of the external force for energy balance to hold for weak solutions of the 2D incompressible Euler equations. This is motivated by turbulence modeling and the result is in contrast with the situation in 3D and the existence of wild solutions.

## [00612] New models and methods for capacity planning and scheduling

**Session Time & Room :**

00612 (1/3) : 1C (Aug.21, 13:20-15:00) @D505

00612 (2/3) : 1D (Aug.21, 15:30-17:10) @D505

00612 (3/3) : 1E (Aug.21, 17:40-19:20) @D505

**Type :** Proposal of Minisymposium

**Abstract :** Scheduling theory has received a wide coverage in the literature on operations research and discrete optimization over the last five decades or so, but the literature seems to have reached a "sink" equilibrium with respect to the standard assumptions and parameters to be included in the models. In this symposium we aim to present recent new scheduling models that extend the classic ones, and where the extensions have a direct link with practical operations scheduling in a variety of industries. We focus especially also on computational methods for solving the new models.

**Organizer(s) :** Roel Leus, Norbert Trautmann

**Classification :** 90B35, 90B36, 90C27, 90C11

**Minisymposium Program :**

00612 (1/3) : 1C @D505 [Chair: Roel Leus]

## [01483] Joint replenishment combined with machine scheduling: offline and online algorithms

**Format :** Talk at Waseda University

**Author(s) :** Tamás Kis (SZTAKI) Peter Gyorgyi (SZTAKI) Timea Tamasi (SZTAKI) Jozsef Bekesi (University of Szeged)

**Abstract :** In this scheduling problem, each job requires a subset of resource types that have to be purchased after the release date of the job and prior to starting the job. The goal is to determine a schedule along with the purchasing dates and quantities for each resource type to minimize the sum of purchasing costs plus a scheduling criterion.

Complexity results and online algorithms will be presented for different special cases of the problem.

## [01552] Sequential testing in batches with resource constraints

**Format :** Talk at Waseda University

**Author(s) :** Fan Yang (Shanghai Normal University)Ben Hermans (ORTEC)Nicolas ZUFFEREY (University of Geneva)Roel Leus (KU Leuven)

**Abstract :** We consider the problem of determining the state of a system through costly tests of its components, where components can be tested simultaneously in batches to exploit economies of scale. This problem is a generalization of the classical sequential testing problem and it has applications in various settings, including machine maintenance, disease diagnosis, and new product development. We prove that the problem is strongly NP-hard, and several models and algorithms are proposed for it.

## [00764] A flow-based formulation for parallel machine scheduling using decision diagrams

**Format :** Talk at Waseda University

**Author(s) :** Daniel Kowalczyk (KU Leuven)Roel Leus (KU Leuven)Christopher Hojny (Eindhoven University of Technology)Stefan Ropke (Technical University of Denmark)

**Abstract :** We present a new flow-based formulation for identical parallel machine scheduling, which is constructed with the help of a decision diagram that represents all job sequences that respect specific ordering rules. These rules rely on a partition of the planning horizon into, generally non-uniform, periods. We develop a branch-and-price framework that solves several instances from the literature for the first time. We compare the new formulation with the time-indexed and arc-time-indexed formulation.

## [00808] Parallel Machine Scheduling Under Uncertainty: Models and Exact Algorithms

**Format :** Online Talk on Zoom

**Author(s) :** Guopeng Song (National University of Defense Technology)Roel Leus (KU Leuven)

**Abstract :** We study parallel machine scheduling for makespan minimization with uncertain job processing times. To incorporate uncertainty and generate solutions that are insensitive to unfolding information, three different modeling paradigms are adopted: a robust model, a chance-constrained model, and a distributionally robust chance-constrained model. We focus on devising generic solution methods that can efficiently handle these different models. We compare the solutions from the different models for scheduling under uncertainty and report the general lessons learned.

00612 (2/3) : 1D @D505 [Chair: Shunji Tanaka]

## [02307] Energy-aware flow shop scheduling with uncertain renewable energy

**Format :** Talk at Waseda University

**Author(s) :** Morteza DAVARI (SKEMA Business School)Masoumeh Ghorbanzadeh (Ferdowsi University)Mohammad Ranjbar (Ferdowsi University)

**Abstract :** This paper investigates an energy-aware flow shop scheduling problem with on-site renewable and grid energy resources. To deal with the uncertainty of renewable energy resources, we first develop two two-stage stochastic programming formulations to minimize the total energy cost purchased from the grid and then, we develop two robust models. Computational results reveal that Benders decomposition algorithms outperform compact models for robust problems and not for stochastic problem.

## [02657] An effective model-driven heuristic algorithm for the collaborative operating room scheduling problem

**Format :** Talk at Waseda University

**Author(s) :** Yang Wang (School of Management, Northwestern Polytechnical University)Haichao Liu (School of Management, Northwestern Polytechnical University)Abraham Punnen (Simon Fraser University)

**Abstract :** In this work, we study a collaborative operating room scheduling problem subject to shared surgeons and downstream wards. We propose an effective model-driven heuristic algorithm to make both weekly surgery assignment and daily sequencing decisions for multiple heterogeneous hospitals. Extensive experimental results disclose the merit of the integrated optimization modelling and the usefulness of coordinating the allocation of key resources within collaborative hospitals.

## [01493] Valid inequalities for the parallel stack loading problem of minimizing the number of badly-placed items

**Format :** Talk at Waseda University

**Author(s) :** Shunji Tanaka (Kyoto University)Sven Boge (Osnabrück University)

**Abstract :** This study addresses the parallel stack loading problem to find an optimal loading plan of incoming items into parallel stacks so that the workload for retrieving them later is minimized. We propose valid inequalities for an integer programming formulation of the problem to minimize the number of badly-placed items as an index of the workload. We examine their effectiveness by computational experiment.

## [01466] Branch-and-Price-and-Cut for the Team Orientation Problem with Interval-Time-Varying Profit

**Format :** Online Talk on Zoom

**Author(s) :** jiaojiao li (National University of Defense Technology)

**Abstract :** This paper studies the team orienteering problem, where the profit depends on whether two visits are completed and the interval time of the two visits. The result of this interaction can be expressed as a discrete profit function. In the practical application of Earth observation satellites, it is often necessary to make two consecutive observations of some important targets at reasonable intervals to improve the observation effect. To solve the problem, we effectively describe the time interval requirement by the number of days between two visits and the combination of time windows, then formulate mixed-integer programming (MIP) models and propose a branch-and-price-cut algorithm, along with valid inequalities for tightening the upper bound. Computational results show the effectiveness of our algorithm. Furthermore, we analyze the impact of the following four aspects on computing time, including basic and modified graph, unidirectional and bidirectional label-setting, ng-path relaxation and dynamic ng-path relaxation, algorithms with and without the valid inequality. Then we present the impact of the third level of branching and non-branching on computing time and profit.

00612 (3/3) : 1E @D505 [Chair: Norbert Trautmann]

## [03681] A hybrid algorithm of integrated container truck scheduling problem

**Format :** Talk at Waseda University

**Author(s) :** Wenchao Wei Yanrong Zhang (Beijing Jiaotong University)

**Abstract :** This article establishes an inland container transportation network that includes inland container depots (ICDs) and studies the dispatching problem of container empty containers and trucks in the network. A mixed integer programming model is proposed to tackle the scheduling problem together with ICD locations. To solve the proposed problem, we develop a hybrid algorithm combining large neighborhood search in a fix-and-optimize framework and a tabu search algorithm.

## [05024] Compact formulations for parallel machine scheduling with conflicts

**Format :** Talk at Waseda University

**Author(s) :** Phablo Moura (KU Leuven)Roel Leus (KU Leuven)Hande Yaman (KU Leuven)

**Abstract :** Parallel machine scheduling with conflicts consists in, given a set of jobs  $V$  with known processing times, a set of identical machines  $M$ , and an undirected graph  $(V, E)$ , finding a mapping from  $V$  to  $M$  such that pairs of jobs in  $E$  are assigned to different machines, and the maximum completion time (makespan) is minimized. We present compact MILP formulations, introduce classes of valid inequalities, and report on preliminary computational experiments

## [01311] Project scheduling under various resource constraints

**Format :** Talk at Waseda University

**Author(s) :** Nicklas Klein (University of Bern)Mario Gnägi (University of Bern)Norbert Trautmann (University of Bern)

**Abstract :** The execution of a project often requires two types of resources: renewable resources representing, e.g., staff members or equipment; and production and consumption resources representing, e.g., the project budget. We present a mixed-integer linear programming formulation for scheduling such a project which significantly outperforms state-of-the-art models from the literature.

# [00615] Nonlinear PDEs & Probability

**Session Time & Room :**

00615 (1/2) : 5B (Aug.25, 10:40-12:20) @G710

00615 (2/2) : 5C (Aug.25, 13:20-15:00) @G710

**Type :** Proposal of Minisymposium

**Abstract :** The aim of this mini-symposium is to present recent results in analysis and probability with applications to the study of nonlinear PDEs relating to mathematical physics, kinetic theory, and fluid mechanics. This includes questions of regularity and irregularity, stability, and geometric properties of solutions.<sup>[1]</sup> We want to bring together young researchers and specialists to foster scientific exchange and explore new exciting developments in the fields.

**Organizer(s) :** Tatsuya Miura, Tobias Ried, Jonas Sauer

**Classification :** 35R60, 35K55, 35Q82, 60H17

**Minisymposium Program :**


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00615 (1/2) : 5B @G710 [Chair: Tobias Ried]

## [04215] A mixed-norm estimate of two-particle reduced density matrix of many-body Schrödinger dynamics for deriving Vlasov equation

**Format :** Talk at Waseda University

**Author(s) :** Li Chen (Universität Mannheim)

**Abstract :** We re-examine the combined semi-classical and mean-field limit in the N-body fermionic Schrödinger equation with pure state initial data using the Husimi measure framework. The Husimi measure equation involves three residue types: kinetic, semiclassical, and mean-field. The main result of this paper is to provide better estimates for the kinetic and mean-field residue than those in the authors' previous work. Especially, the estimate for the mean-field residue is shown to be smaller than the semiclassical residue by a mixed-norm estimate of the two-particle reduced density matrix factorization. Based on this estimate, we find that the mean-field residue is of higher order than the semiclassical residue. The talk is based on the joint work with Jinyeop Lee, Matthew Liew, and Yue Li.

## [03911] Hydrodynamic limit equations derived from microscopic interacting particle systems

**Format :** Talk at Waseda University

**Author(s) :** Makiko Sasada (University of Tokyo)

**Abstract :** Hydrodynamic limit provides a rigorous mathematical method to derive the deterministic partial differential equations describing the time evolution of macroscopic parameters, from the stochastic dynamics of a microscopic large scale interacting system. In this talk, by introducing the notion of a class of valid interacting particle systems, and we discuss what kind of equations can be derived from such interacting particle systems.

## [01645] The Vicsek-BGK equation in collective dynamics

**Format :** Talk at Waseda University

**Author(s) :** Raphael Winter (University of Vienna)

**Abstract :** The Vicsek-BGK equation describes the collective motion of agents with local alignment. It is known that the spatially homogeneous model undergoes a phase transition from disoriented motion to collective motion. In this contribution we give a prove the onset of a phase transition in the spatially inhomogeneous case. Joint work with Sara Merino Aceituno and Christian Schmeiser.

## [03240] Quasilinear SPDEs with rough paths

**Format :** Talk at Waseda University

**Author(s) :** Alexandra Neamtu (University of Konstanz)Antoine Hocquet (Technical University of Berlin)

**Abstract :** We investigate quasilinear parabolic evolution equations driven by a  $\gamma$ -Hölder rough path, where  $\gamma \in (1/3, 1/2]$ . This includes the Brownian motion and a fractional Brownian motion with Hurst index  $H \in (1/3, 1/2]$ . We explore the mild formulation combining functional analytic techniques with the controlled rough paths approach. We apply our results to the stochastic Landau-Lifshitz-Gilbert equation for which we additionally prove the existence of stochastic flows. This talk is based on a joint work with Antoine Hocquet.

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00615 (2/2) : 5C @G710 [Chair: Jonas Sauer]

**[03798] A regularity structure for the quasilinear generalized KPZ equation****Format :** Talk at Waseda University**Author(s) :** Masato Hoshino (Osaka University)Ismael Bailleul (Universite Rennes 1)Seiichiro Kusuoka (Kyoto University)**Abstract :** We prove the local well-posedness of a regularity structure formulation of the quasilinear generalized KPZ equation and give an explicit form of the renormalized equation in the full subcritical regime.**[03415] Gradient continuity of weak solutions for perturbed one-Laplace problems****Format :** Talk at Waseda University**Author(s) :** Shuntaro Tsubouchi (Graduate School of Mathematical Sciences, University of Tokyo)**Abstract :** This talk is concerned with continuity of a spatial derivative of weak solutions to very singular problems that involve both one-Laplace and  $p$ -Laplace operators. The main difficulty is that one-Laplacian has both singular and degenerate ellipticity, which makes it difficult to prove Hölder continuity of a spatial gradient across a facet, the degenerate region of a gradient. In this talk, the speaker would like to talk about recent results on gradient continuity across the facet.**[02739] Asymptotic behavior of geometric flows with contact angle conditions****Format :** Talk at Waseda University**Author(s) :** Takashi Kagaya (Muroran Institute of Technology)**Abstract :** Several geometric flows were derived from interface phenomena. In this talk, contact angle conditions for the geometric flows are dealt with, motivated by surface tension problems. The asymptotic behavior of the geometric flows depends on the contact angle conditions. In particular, traveling waves have the asymptotic stability if we assume specific contact angle conditions. I will introduce my results related to the asymptotic behavior.**[05334] Weak-strong uniqueness for volume-preserving mean curvature flow****Format :** Online Talk on Zoom**Author(s) :** Tim Laux (University of Bonn)**Abstract :** I will discuss a stability and weak-strong uniqueness principle for volume-preserving mean curvature flow. The proof is based on a new notion of volume-preserving gradient flow calibrations, which is a natural extension of the concept in the case without volume preservation recently introduced by Fischer et al. [arXiv:2003.05478]. The first main result shows that any strong solution with certain regularity is calibrated. The second main result consists of a stability estimate in terms of a relative entropy, which is valid in the class of distributional solutions to volume-preserving mean curvature flow.**[00616] Continuous optimization: theoretical and algorithmic trends****Session Time & Room :**

00616 (1/3) : 1E (Aug.21, 17:40-19:20) @A207

00616 (2/3) : 2C (Aug.22, 13:20-15:00) @A207

00616 (3/3) : 2D (Aug.22, 15:30-17:10) @A207

**Type :** Proposal of Minisymposium**Abstract :** Continuous optimization is one of the main areas in Applied Mathematics. It has plentiful applications and rich theory and algorithms. This mini-symposium presents recent advances in the area, starting from important theoretical aspects of optimality conditions that guide the development of different algorithms based on higher order information, like Newton-type and third-order algorithms. Many of the methods also exploit the specific structure of the underlying application to achieve high performance. Finally, the mini-symposium also pays tribute to José Mario Martínez's influence in the field. The contributions can be somewhat linked to his insightful ideas in different periods of his career.**Organizer(s) :** Paulo J. S. Silva, Roberto Andreani

**Classification :** 90C30**Minisymposium Program :**

00616 (1/3) : 1E @A207 [Chair: Paulo J. S. Silva]

## [03840] Constant rank constraint qualification for nonlinear second-order cone programming

**Format :** Talk at Waseda University**Author(s) :** Gabriel Haeser (University of Sao Paulo)

**Abstract :** We revisit the classical notions of nondegeneracy and Robinson's condition in the context of nonlinear second-order cone programming. For an m-dimensional second-order cone, instead of stating nondegeneracy at the vertex as the linear independence of m derivative vectors, we do it in terms of several statements of linear independence of two derivative vectors. This allows embedding the structure of the second-order cone into the formulation of the conditions, providing weaker variants and applications.

## [03851] Strong global convergence properties of an Augmented Lagrangian method for symmetric cones

**Format :** Talk at Waseda University**Author(s) :** Daiana Oliveira dos Santos (UNIFESP)

**Abstract :** Sequential optimality conditions have played a major role in proving stronger global convergence results for numerical algorithms used in nonlinear programming. Several extensions have been described in conic contexts, leading to many open questions. In this talk, we will present new sequential optimality conditions for nonlinear symmetric cone programming. Stronger results are obtained by exploiting the rich algebraic structure of the problem.

## [02990] On enhanced KKT optimality conditions for smooth nonlinear optimization

**Format :** Talk at Waseda University**Author(s) :** Roberto Andreani (State University of Campinas/ UNICAMP)

**Abstract :** The Fritz-John and Karush-Kuhn-Tucker (KKT) conditions are crucial for finding minimizers in constrained optimization. They have been augmented with extra necessary conditions since the 1970s, with the enhanced KKT stationarity being one of them. This work focuses on enhanced KKT stationarity for smooth nonlinear programming and analyzes improved multipliers with quasi-normality. The results have implications for sequential optimality conditions and complementarity constraints in multi-objective problems.

00616 (2/3) : 2C @A207 [Chair: Stefania Bellavia]

## [03586] Adaptive Third-Order Methods for Composite Convex Optimization

**Format :** Talk at Waseda University**Author(s) :** Geovani Grapiglia (UCLouvain)Yurii Nesterov (UCLouvain)

**Abstract :** In this talk we present adaptive third-order methods for composite convex optimization problems in which the smooth part has Lipschitz continuous third-order derivatives. In our new schemes the regularization parameters are tuned by checking the progress of the inner solver used to compute trial points. In particular, this technique allows us to design an adaptive accelerated method that can find an  $\epsilon$ -approximate solution using at most  $\mathcal{O}(|\log(\epsilon)|\epsilon^{-\frac{1}{4}})$  iterations of the inner solver.

## [03706] On the globalization of nonlinear programming methods.

**Format :** Talk at Waseda University**Author(s) :** L. Felipe Bueno (Universidade Federal de São Paulo)

**Abstract :** In this work we identify some very general conditions that guarantee the global convergence of numerical methods to solve constrained nonlinear optimization problems. With that in mind, we show that a range of Inexact Restoration methods fit the presented framework. Furthermore, we propose a particular algorithm in this line, combined with an acceleration process supported by the general theory of convergence. Computational tests attest to the efficiency of the proposed strategy.

## [04137] Proportionality based algorithms for quadratic programming

**Format :** Talk at Waseda University

**Author(s) :** Gerardo Toraldo (Università della Campania "L.Vanvitelli")William W. Hager (University of Florida)Marco Viola (University College Dublin)

**Abstract :** We present a decomposition of the negative gradient on the tangent cone at a feasible point for optimization problems with polyhedral constraints. This decomposition, based on the idea of proportioning, extends the definition of the free and chopped gradient in bound constrained optimization. Such decomposition allows us to generalize the definition of binding variables and to measure complementary aspects of stationarity that can be exploited to design effective switching rules in Gradient Projection two-phase algorithms.

00616 (3/3) : 2D @A207 [Chair: Roberto Andreani]

## [03943] On the Inexact Restoration approach for adaptive sample size in finite sum minimization

**Format :** Talk at Waseda University

**Author(s) :** Stefania Bellavia (University of Florence)Natasa Krejic (University of Novi Sad)Benedetta Morini (University of Florence)Simone Rebegoldi (University of Florence)

**Abstract :** In this talk we discuss recent advances in the inexact restoration approach combined with stochastic trust-region methods for finite-sum minimization problems. At each iteration, the proposed methods approximate the function and the derivatives by subsampling. The choice of the function sample size is ruled by the Inexact Restoration approach, whereas the derivatives approximations are computed averaging in smaller sets.

We report worst-case complexity results in expectation and numerical results showing the advantages of adaptive approaches.

## [03290] Block coordinate descent and the close enough traveling salesman problem

**Format :** Talk at Waseda University

**Author(s) :** Ernesto G. Birgin (University of São Paulo)

**Abstract :** At each iteration of a Block Coordinate Descent method one minimizes a constrained approximation of the objective function with respect to a generally small set of variables. In this work we address the problem in which block constraints are not defined by global sets of equations and inequations. An algorithm is defined and convergence and complexity are proved. The proposed method is used to solve a generalization of the close enough traveling salesman problem.

## [02948] Sequential optimality conditions: how to stop optimization algorithms

**Format :** Talk at Waseda University

**Author(s) :** Paulo J. S. Silva (University of Campinas)

**Abstract :** Optimality conditions, like KKT, play essential roles in modern optimization. They may be used as a starting point to develop algorithms or as a condition to accept an approximate solution. This dynamic aspect, led to the development of sequential optimality conditions that try to capture the iterative approximation nature of computed sequences. In this talk, we will present how this development enlightened the convergence requirements and termination criteria of algorithms in nonlinear optimization.

## [01945] Distributed Inexact Newton Method with Adaptive Step Sizes

**Format :** Talk at Waseda University

**Author(s) :** Natasa Krejic (University of Novi Sad)Dusan Jakovetic (University of Novi Sad)Greta Malaspina (University of Novi Sad)

**Abstract :** We consider distributed personalized optimization and consensus optimization and propose DINAS - Distributed Inexact Newton method with Adaptive Stepsize. DINAS employs large adaptive step-sizes, requires a reduced global parameters knowledge with respect to existing alternatives and does not need any local Hessian inversion nor Hessian communications. The method achieves quadratic convergence with respect to computational cost and linear convergence with respect to communication cost for personalized optimization and global convergence for consensus optimization.

# [00621] Frontiers of Collaboration with Industry: Succeeding through Failure

## **Session Time & Room :**

00621 (1/2) : 3D (Aug.23, 15:30-17:10) @G406

00621 (2/2) : 3E (Aug.23, 17:40-19:20) @G406

## **Type :** Proposal of Industrial Minisymposium

**Abstract :** Corresponding to the organizational efforts introduced in the mini-symposium “Frontiers of Collaboration with Industry: Towards International Mathematical Commons,” this mini-symposium introduces diverse efforts at practical research activities that engage mathematicians, together with companies, to solve specific problems. With a spirit of collaboration, we aim at sharing with participants some issues and challenges at the forefront of mathematical science research, a collaborative system with companies, and various mathematical ideas for application to problem-solving. Through collaboration between industry and mathematical science, all are intended for the successful resolution of the many issues which must be addressed by our society.

**Organizer(s) :** Takashi Sakajo, Kenji Kajiwara, Hiroshi Suito

**Classification :** 74-10, 76-10, 78-10, Applications to industrial problems

## **Minisymposium Program :**

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00621 (1/2) : 3D @G406 [Chair: Takashi Sakajo]

## **[01441] Mobility Optimization Engine and its Real-world Applications**

### **Format :** Talk at Waseda University

**Author(s) :** Katsuki Fujisawa (Kyushu University)

**Abstract :** Various efforts have been made to realize a so-called super-smart society recently. Our project team builds services to create new industries and other services through corporate collaboration. We have utilized large-scale computing infrastructures and developed the Cyber-Physical System Mobility Optimization Engine (CPS-MOE) that provides various functions, including creating new industries. It can reduce cost and industrial waste and constructing services to calculate the optimum control schedule of transportation agencies. The latest research results and industry-academia collaborative projects using CPS-MOE will be presented in this talk.

## **[02078] Mathematical modeling with industry in the water sector: what makes good practice**

### **Format :** Talk at Waseda University

**Author(s) :** Anthony John Jakeman (Australian National University)

**Abstract :** We emphasize the role of good practices in conducting an integrated assessment exercise in water availability settings, underlining attention throughout the framing, assessment and engagement steps. We stress the notion of reflexivity on pathway decisions at each decision fork in the exercise and a holistic attention to uncertainty sources throughout the process, not just in the formulated models. These aspects will be illustrated with a case study in a catchment of the Murray-Darling Basin.

## **[01474] An international research program on industrial problems for math students.**

### **Format :** Talk at Waseda University

**Author(s) :** Hiroshi Suito (Tohoku University)

**Abstract :** In this talk, a student research program with industrial projects in mathematics, called “g-RIPS-Sendai”, which has been held in Japan since 2018 is introduced. This program offers graduate students in mathematics stimulating opportunities to work on realistic research projects provided by industries. For industrial partners, this program provides chances to try new mathematical approaches with fresh ideas from young students. Our experiences including several difficulties will be shared and discussed.

## [02098] Collaboration with early graduate researchers, and improvements on simulated annealing

**Format :** Talk at Waseda University

**Author(s) :** Joseph David (University of Washington)Kemal Aziez Rachmansyah (Tohoku University)Rikuto Shigemi (University of Tsukuba)Zachary Brennan (Iowa State University)

**Abstract :** Students with a pure mathematics background can struggle to find early opportunities in industry without the correct guidance. As opposed to traditional graduate internships which may expect certain familiarity with industry-related problems, a hybrid academic-industry approach with both academic and industry mentors can provide a bridge for early graduate students wishing to transition to industry. This talk discusses the pros and cons of one such program from the perspective of a mid-career graduate student.

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00621 (2/2) : 3E @G406 [Chair: Hiroshi Suito]

## [02914] Development of a CNN-Based Model for Car Classification and Damage Detection from car accidents

**Format :** Talk at Waseda University

**Author(s) :** Busayamas pimpunchat (King Mongkut's Institute of Technology Ladkrabang)

**Abstract :** This study aimed to develop a convolutional neural network (CNN)-based model for car classification and damage detection from car accidents. The research found that the model was highly accurate in classifying the position of a single car and detecting damage and the model's performance in detecting multiple cars, a modified version of the Hough Transform algorithm was used to improve. The study's findings can help insurance companies analyze car damage and introduce relevant sections in vehicle regulations.

## [03805] Failure and Success for Bauxite Moisture Measurement with Microwaves

**Format :** Talk at Waseda University

**Author(s) :** Mark Joseph McGuinness (Victoria University of Wellington)Lata I Paea (University of the South Pacific)Sione Paea (University of the South Pacific)

**Abstract :** The weight of bauxite ore is strongly dependent on moisture content. A microwave analyser measures phase and attenuation in real time, to infer moisture content, which directly impacts the price paid per tonne. Simple linear models fail to explain the highly nonlinear dependence on bauxite depth that is seen in attenuation data. Motivated by this failure, we develop a successful four-layer model that allows multiple reflections at interfaces between ore and air.

## [02161] The UniSA Mathematics Clinic: Renewables, defence, mining, drones, and justice

**Format :** Talk at Waseda University

**Author(s) :** Lesley Ann Ward (University of South Australia)

**Abstract :** The University of South Australia Mathematics Clinic runs yearlong authentic industry-sponsored research projects for small teams of final-year undergraduate mathematics students. Clinic projects give students professional skills, experience, accomplishments, and employability, and generate research progress and publications. But things can go wrong – with sponsors, students, staff, projects, workload, and logistics. How can we minimise things going wrong, and fix them when they do? I'll offer some case studies, suggestions, and principles, drawn from Clinic experience.

## [01470] Interdisciplinary research using Topological Flow Data Analysis through Math Clinic

**Format :** Talk at Waseda University

**Author(s) :** Takashi Sakajo (Kyoto University)

**Abstract :** Topological Flow Data Analysis "TFDA" is a new way of data analysis based on the classification theory of 2D vector fields. It extracts and quantifies topological features of complex flows from various datasets efficiently. We are organizing a research platform, called Math Clinic, at Kyoto University, where interdisciplinary research with other disciplines including industry has been conducted based on TFDA. In this talk, we will report on the activity and results of the Math Clinic.

# [00622] Inverse Problems and Imaging

**Session Time & Room :**

00622 (1/3) : 1C (Aug.21, 13:20-15:00) @E605

00622 (2/3) : 1D (Aug.21, 15:30-17:10) @E605

00622 (3/3) : 1E (Aug.21, 17:40-19:20) @E605

**Type :** Proposal of Minisymposium

**Abstract :** Inverse problems are concerned with determining unknown parameters of interest from indirect, partial, and noisy measurements with the aid of a mathematical model. Such problems are fundamental in biomedical imaging, non-destructive testing, and modern astronomy. Often, these parameters take the form of images rather than scalar or vector-valued parameters, requiring special methods adapted to the distributed structure. The aim of this minisymposium is to gather an active group of researchers working on variational methods for solving inverse and imaging problems, in order to foster increased interaction between these fields and those of applications in science, technology, and industry.

**Organizer(s) :** Christian Clason

**Classification :** 65J22, 92C55, inverse problems; mathematical imaging; medical imaging; non-destructive testing

**Minisymposium Program :**


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00622 (1/3) : 1C @E605 [Chair: Clason]

## [01259] Testing statistical hypothesis in Inverse Problems

**Format :** Talk at Waseda University

**Author(s) :** Frank Werner (Universität Würzburg)Remo Kretschmann (Universität Würzburg)Daniel Wachsmuth (Universität Würzburg)

**Abstract :** In this talk, we propose a regularized approach to hypothesis testing in Inverse Problems in the sense that the underlying estimators or test statistics are allowed to be biased. As one major result we prove that regularized testing is always at least as good as classical unregularized testing. We furthermore provide an adaptive test by maximizing the power functional, which outperforms unregularized tests in numerical simulations by several orders of magnitude.

## [01346] Disentangling domain bias in medical images for meaningful embeddings

**Format :** Talk at Waseda University

**Author(s) :** Samuel Tull (University of Cambridge)

**Abstract :** Machine learning models using imaging have been promising to revolutionise healthcare for many years but are rarely deployed in the clinic due to underlying dataset biases and distribution shifts. In medical images, several sources of bias cause a distribution shift: image acquisition protocols, the instrument used and any image processing. We discuss a method giving meaningful image embeddings, useful for downstream tasks, that have been disentangled from sources of bias, achieving improved generalisability and interpretability.

## [01553] A Bregman-Kaczmarz method for nonlinear systems of equations

**Format :** Talk at Waseda University

**Author(s) :** Maximilian Winkler (TU Braunschweig)

**Abstract :** We propose a new randomized method for solving systems of nonlinear equations for sparse solutions or solutions which are subject to simple additional constraints. The method uses only gradients of component functions and is based on Bregman projections. Convergence is established for convex nonnegative functions and for functions that fulfill the local tangential cone condition. We demonstrate in examples that the method can find sparse or simplex-constrained solutions of inverse problems.

## [01556] A complementary $\ell^1$ -TV reconstruction algorithm for limited data CT

**Format :** Talk at Waseda University

**Author(s) :** Simon Goeppl (University of Innsbruck)Jürgen Frikel (OTH Regensburg)Markus Haltmeier (University of Innsbruck)

**Abstract :** In this talk, we introduce a new variational reconstruction framework for inverse problems, suffering from incomplete data. As it is known that a single regularizer does not work flawlessly for noise reduction and artifact removal simultaneously, we instead address both problems by subsequent reconstructions. These reconstructions are connected by a data-consistency term, which enables us to utilize both properties of  $\ell_1$ -curvelet and total variation regularization in the example of limited angle tomography.

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00622 (2/3) : 1D @E605 [Chair: Frank Werner]

## [01577] 3D image reconstruction for cone beam computed tomography using sparsity

**Format :** Talk at Waseda University

**Author(s) :** Alexander Meaney (University of Helsinki)Samuli Siltanen (University of Helsinki)

**Abstract :** Cone beam computed tomography is an increasingly popular three-dimensional medical imaging technique. However, in many settings it suffers from suboptimal image quality. In this work, we will present a new approach to regularized iterative image reconstruction. Our technique has an in-built automatic choice of the regularization parameter, based on a priori knowledge on gradient sparsity. Combined with a novel primal-dual optimization algorithm, this results in an efficient technique for large-scale reconstruction of improved quality.

## [01591] High Dynamic Range Tomography via Modulo Radon Transform

**Format :** Talk at Waseda University

**Author(s) :** Matthias Beckmann (University of Bremen)

**Abstract :** Recently, practitioners in tomography proposed high dynamic range solutions that are inspired by multi-exposure fusion strategies in computational photography. In this talk, we propose a single-shot alternative based on the novel Modulo Radon Transform, which folds Radon projections via modulo non-linearity into the dynamic range of the sensor to avoid information loss due to saturation. We propose a sequential reconstruction algorithm, which is backed by mathematical guarantees, and illustrate our theoretical results by numerical simulations.

## [01593] A new inversion scheme for elastic diffraction tomography

**Author(s) :** Bochra Mejri (RICAM, Austria) Johann Radon Institute for Computational and Applied Mathematics)Otmar Scherzer (University of Vienna)

**Abstract :** We consider the problem of elastic diffraction tomography, which consists in reconstructing elastic properties, i.e. mass density and elastic Lamé parameters, of a weakly scattering medium from full-field data of scattered waves outside the medium. Elastic diffraction tomography refers to the elastic inverse scattering problem after linearization using a first-order Born approximation. In this paper, we prove the Fourier diffraction theorem, which relates the 2D Fourier transform of scattered waves with the Fourier transform of the scatterer in the 3D spatial Fourier domain. Elastic wave mode separation is performed, which decomposes a wave into four modes. A new two-step inversion process is developed, providing information on the modes first and secondly on the elastic parameters. Finally, we discuss reconstructions with plane wave excitation experiments for different tomographic setups and with different plane wave excitation frequencies, respectively.

## [01606] inverse electromagnetic scattering problems with internal dipoles

**Format :** Talk at Waseda University

**Author(s) :** Yakun Dong (University of Vienna)Otmar Scherzer (University of Vienna)Kamran Sadiq (Radon Institute for Computational and Applied Mathematics)

**Abstract :** We propose a method to reconstruct the optical properties of inverse scattering problems with internal sources. The method is based on macroscopic Maxwell's equations and achieves super-resolution reconstruction. Applications in single-molecule localization microscopy are shown.

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00622 (3/3) : 1E @E605 [Chair: Clason]

## [03917] A paraxial approach for the inverse problem of vibroacoustic imaging

**Format :** Talk at Waseda University

**Author(s) :** Teresa Rauscher (University of Klagenfurt)

**Abstract :** Vibroacoustography by means of ultrasound is an imaging method that was developed to achieve higher resolutions while avoiding the drawbacks of scattering and stronger attenuation. High frequency waves that show a strongly preferred direction of propagation are sent into the medium. Therefore, we make use of a paraxial approach to arrive at a system of PDEs that involve space dependent parameters. In this talk, we will deal with the modeling and inverse problem for vibroacoustography.

## [05513] Primal-dual proximal splitting and generalized conjugation in non-smooth non-convex optimization

**Format :** Talk at Waseda University

**Author(s) :** Christian Clason (University of Graz)Stanislav Mazurenko (Masaryk University)Tuomo Valkonen (EPN, Quito and University of Helsinki)

**Abstract :** We demonstrate that non-convex non-smooth optimization problems like the Potts segmentation model can be written in terms of generalized conjugates of convex functionals, which can be solved by a conceptually straightforward extension of the primal-dual proximal splitting method of Chambolle and Pock. We show convergence and illustrate these theoretical results numerically on the aforementioned example problem.

## [00624] At the interface between neural networks and differential equations

**Session Time & Room :**

00624 (1/2) : 3C (Aug.23, 13:20-15:00) @E702

00624 (2/2) : 3D (Aug.23, 15:30-17:10) @E702

**Type :** Proposal of Minisymposium

**Abstract :** Deep neural networks have recently been used to design innovative, and arguably revolutionary, methods for solving a large number of challenging problems from science and engineering which are modeled by differential equations. Conversely, differential equations provide an important set of tools for understanding methods based upon neural networks. This minisymposium is dedicated to recent progress at the interface between neural networks and differential equations, including topics such as the theoretical convergence analysis and computation of neural networks for solving high dimensional PDEs in addition to the analysis, training, and design of neural networks using perspectives from the study of differential equations.

**Organizer(s) :** Yulong Lu, Jonathan Siegel, Stephan Wojtowytsh

**Classification :** 65M22, 68W25, Machine Learning

**Minisymposium Program :**

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00624 (1/2) : 3C @E702 [Chair: Yulong Lu]

## [01481] Operator learning and nonlinear model reduction by deep neural networks

**Format :** Talk at Waseda University

**Author(s) :** Wenjing Liao (Georgia Institute of Technology)

**Abstract :** This talk focuses on the problem of operator learning to learn an operator between function spaces from data. Model reduction plays a significant role, to reduce the data dimension and the problem size. We consider a neural network architecture to utilize low-dimensional nonlinear structures in model reduction, and prove an upper bound of the generalization error. Our theory shows that, the sample complexity depends on the intrinsic dimension of the model.

## [01838] A deep learning framework for geodesics under spherical Wasserstein-Fisher-Rao metric

**Format :** Talk at Waseda University

**Author(s) :** Yang Jing (Shanghai Jiao Tong University)

**Abstract :** Wasserstein-Fisher-Rao (WFR) distance is a family of metrics to gauge the discrepancy of two measures. Compared to the case for Wasserstein distance, the understanding of geodesics under spherical WFR is less clear . We develop a deep learning framework to compute geodesics under spherical WFR metric, and the learned geodesics can be adopted to generate weighted samples. Our framework can be beneficial for applications with given weighted samples, especially in Bayesian inference.

## [01927] Mean-field Analysis of Piecewise Linear Solutions for Wide ReLU Networks

**Format :** Talk at Waseda University

**Author(s) :** Marco Mondelli (Institute of Science and Technology Austria (ISTA))

**Abstract :** We consider a two-layer ReLU network trained via SGD for univariate regression. By connecting the SGD dynamics to the solution of a gradient flow, we show that SGD is biased towards a simple solution: at convergence, the ReLU network implements a piecewise linear map of the inputs, and the number of "knot" points - i.e., points where the tangent of the ReLU network estimator changes - between two consecutive training inputs is at most three.

## [02274] On the Mean-field Theory of Neural Network Training

**Format :** Talk at Waseda University

**Author(s) :** Zhengdao Chen (Google)

**Abstract :** To understand the training of wide neural networks, prior studies have considered the infinite-width mean-field limit of two-layer neural networks, whose training dynamics is characterized as the Wasserstein gradient flow of a probability distribution. In this talk, we will present a mean-field theory for a type of three-layer neural networks whose first-layer weights are random and fixed, through which we prove a linear-rate convergence guarantee and generalization bounds.

00624 (2/2) : 3D @E702 [Chair: Yulong Lu]

## [01535] Machine learning for/with Differential Equation Modeling: Statistics and Computation

**Format :** Online Talk on Zoom

**Author(s) :** Yiping Lu (Stanford University)

**Abstract :** Massive data collection and computational capabilities have enabled data-driven scientific discoveries and control of engineering systems. However, there are still several questions that should be answered to understand the fundamental limits of just how much can be discovered with data and what is the value of additional information. For example, 1) How can we learn a physics law or economic principle purely from data? 2) How hard is this task, both computationally and statistically? 3) What's the impact on hardness when we add further information (e.g., adding data, model information)? I'll answer these three questions in this talk in two learning tasks. A key insight in both two cases is that using direct plug-in estimators can result in statistically suboptimal inference.

The first learning task I'll discuss is linear operator learning/functional data analysis, which has wide applications in causal inference, time series modeling, and conditional probability learning. We build the first min-max lower bound for this problem. The min-max rate has a particular structure where the more challenging parts of the input and output spaces determine the hardness of learning a linear operator. Our analysis also shows that an intuitive discretization of the infinite-dimensional operator could lead to a sub-optimal statistical learning rate. Then, I'll discuss how, by suitably trading-off bias and variance, we can construct an estimator with an optimal learning rate for learning a linear operator between infinite dimension spaces. We also illustrate how this theory can inspire a multilevel machine-learning algorithm of potential practical use.

For the second learning task, we focus on variational formulations for differential equation models. We discuss a prototypical Poisson equation. We provide a minimax lower bound for this problem. Based on the lower bounds, we discover that the variance in the direct plug-in estimator makes sample complexity suboptimal. We also consider the optimization dynamic for different variational forms. Finally, based on our theory, we explain an implicit acceleration of using a Sobolev norm as the objective function for training

## [02223] Momentum Based Acceleration for Stochastic Gradient Descent

**Format :** Talk at Waseda University

**Author(s) :** Kanan Gupta (Texas A&M University)Stephan Wojtowytsh (Texas A&M University)Jonathan Wolfram Siegel (Texas A&M University)

**Abstract :** We will discuss first order optimization algorithms based on discretizations of the heavy ball ODE. Particularly, we introduce a discretization that leads to an accelerated gradient descent algorithm, which provably achieves an accelerated rate of convergence for convex objective functions, even if the stochastic noise in the gradient estimates is significantly larger than the gradient. We compare the optimizer's performance with other popular optimizers on the non-convex problem of training neural networks on some standard datasets.

## [03468] The Effects of Activation Functions on the Over-smoothing of GCNs

**Format :** Online Talk on Zoom

**Author(s) :** Bao Wang (University of Utah)

**Abstract :** Smoothness has been shown to be crucial for the success of graph convolutional networks (GCNs); however, over-smoothing has become inevitable. In this talk, I will present a geometric characterization of how activation functions of a graph convolution layer affect the smoothness of their input leveraging the distance of graph node features to the eigenspace of the largest eigenvalue of the (augmented) normalized adjacency matrix, denoted as M. In particular, we show that 1) the input and output of ReLU or leaky ReLU activation function are related by a high-dimensional ball, 2) activation functions can increase, decrease, or preserve the smoothness of node features, and 3) adjusting the component of the input in the eigenspace M can control the smoothness of the output of activation functions. Informed by our theory, we propose a universal smooth control term to modulate the smoothness of learned node features and improve the performance of existing graph neural networks.

## [03523] On the generalization and training of Deep Operator Networks

**Format :** Online Talk on Zoom

**Author(s) :** Yeonjong Shin (North Carolina State University) Sanghyun Lee (Florida State University)

**Abstract :** We propose a novel training method for Deep Operator Networks (DeepONets). DeepONets are constructed by a sum of products of two sub-networks, namely, branch and trunk networks. The goal is to effectively learn DeepONets that accurately approximate nonlinear operators from data. The standard approaches train the two sub-networks simultaneously via first-order optimization methods. The proposed method, however, trains trunk networks first based on norm-minimization, and then trains branch networks in sequence. Furthermore, we estimate a generalization error of DeepONets in terms of the numbers of training data, sensors in inputs and outputs, and DeepONet size. Several numerical examples including Darcy flow in heterogeneous porous media are presented to illustrate the effectiveness of the proposed training method.

# [00625] Mathematical Modeling and Combinatorial Optimization

**Session Time & Room :**

00625 (1/2) : 4C (Aug.24, 13:20-15:00) @D501

00625 (2/2) : 4D (Aug.24, 15:30-17:10) @D501

**Type :** Proposal of Minisymposium

**Abstract :** Combinatorial optimization problems aim to compute optimal solutions under a series of constraints, where the set of feasible solutions is discrete, such as scheduling and routing problems. It involves thousands of real-world problems. This minisymposium will focus on mathematical modeling and combinatorial optimization. We have eight junior and senior researchers giving their latest research results on algorithm design, modeling of real-world problems and simulation. The purpose of this minisymposium is to discuss new ideas and challenging problems, as well as to explore new research topics.

**Organizer(s) :** Yannan Hu

**Classification :** 90C27

**Minisymposium Program :**

00625 (1/2) : 4C @D501 [Chair: Wei Wu]

## [02230] Sports Scheduling: Number of Trips in the Traveling Tournament Problem

**Format :** Talk at Waseda University

**Author(s) :** Takaki Ono (Chuo University) Shinji Imahori (Chuo University)

**Abstract :** This talk deals with the traveling tournament problem, which is a well-known benchmark problem in the field of sports scheduling. We propose a new technique to improve the efficiency of an existing algorithm for the problem. We also design a new method to improve the quality of solutions. Our method first solves an integer programming problem to compute a round-robin tournament, and constructs a double round-robin tournament with smaller number of trips.

## [04421] Efficient allocation of demand to facilities on road networks

**Format :** Talk at Waseda University

**Author(s) :** Ken-ichi Tanaka (Keio University)Mutsunori Yagiura (Nagoya University)

**Abstract :** We focus on road networks in which some facilities exist and demand for deliveries arises along the edges of the network. We consider the problem of assigning a subset of edges to each facility so that the total facility-demand delivery distances are minimized with the constraint that each facility addresses almost the same amount of demand. We propose an approach to obtain simple and geographically compact service areas by iteratively solving integer optimization problems.

## [01600] Optimal UAV Flight Path Planning for Herding Sheep

**Format :** Talk at Waseda University

**Author(s) :** I-Lin Wang (Professor)Ying-Ting Lin (Ph.D. student)

**Abstract :** We will first introduce how literature solves the shepherding problem by autonomous agents. All the previous research designed heuristic algorithms to collect the sheep when they are too dispersed and then drive them to the destination after aggregating them. We, on the other hand, propose an innovative framework based on graph theory and integer programming models. Our approaches have a significant performance improvement and provide a new viewpoint on how this problem can be solved.

## [02992] Formulations and algorithms for a square independent packing problem

**Format :** Talk at Waseda University

**Author(s) :** Wei Wu (Shizuoka University)Hiroki Numaguchi (Tokyo University of Science)Jotaro Kuno (Nagoya University)Yannan Hu (Tokyo University of Science)Vitor Mitsuo Fukushige Hama (Nagoya University)Mutsunori Yagiura (Nagoya University)

**Abstract :** Given a set of squares and a strip with a fixed width, we consider a square independent packing problem (SIPP) that minimizes the strip height such that all squares are packed into cells by setting vertical and horizontal dividers that pass through the entire strip. We show that the SIPP is NP-hard. To solve the SIPP, we design three mathematical formulations based on different solution representations, and then we propose a fully polynomial-time approximation scheme.

00625 (2/2) : 4D @D501 [Chair: Kazuki Hasegawa]

## [02859] A core selection method for the robust traveling salesman problem

**Format :** Talk at Waseda University

**Author(s) :** Kazuki Hasegawa (Shizuoka University)Wei Wu (Shizuoka University)Mutsunori Yagiura (Nagoya University)

**Abstract :** We consider the robust traveling salesman problem with interval costs under a min–max regret criterion. We first show that the iterated dual substitution method is applicable for solving this problem, and we examine 18 implementations based on different cut generation rules and mathematical models of the classical traveling salesman problem. Then, we propose a new heuristic approach: core selection method. The core selection method achieved state-of-the-art results on all benchmark instances.

## [02909] Algorithms for two-machine job-shop scheduling problem with one joint job

**Format :** Talk at Waseda University

**Author(s) :** Hiroki Numaguchi (Tokyo University of Science)Wei Wu (Shizuoka University)Yannan Hu (Tokyo University of Science)

**Abstract :** We introduce a two-machine job-shop scheduling problem with one joint job where a joint job is defined as a job whose operations are to be processed by different machines. We prove that this problem is strongly NP-hard and propose a polynomial-time algorithm based on dynamic programming when the number of jobs is given as a fixed number. We further improve time complexity using various techniques, including the two-pointers method.

## [04538] A New Multivariate Decision Tree Based on Mixed Integer Linear Programming

**Format :** Talk at Waseda University

**Author(s) :** Ryo Kurosu (University of Kyoto)Kazuya Haraguchi (University of Kyoto)

**Abstract :** We study a novel framework of inferring molecule structures that are expected to have desired properties (e.g., high boiling point, low solubility), exploiting machine learning and operations research, where accurate prediction tools are indispensable. In this paper, we propose a new classification decision tree algorithm that builds a multivariate decision tree (i.e., node split is done by hyperplane) based on mixed integer linear programming. Our algorithm is a generalization of conventional ones in the sense that their decision trees are univariate. We describe experimental results on how accurate decision trees are built by our algorithm and by conventional ones, using data sets from cheminformatics.

## [04561] A Linear Delay Algorithm for Enumeration of 2-Edge/Vertex-connected Induced Subgraphs

**Format :** Talk at Waseda University

**Author(s) :** Takumi Tada (Graduate School of Informatics, Kyoto University, Japan)Kazuya Haraguchi (Graduate School of Informatics, Kyoto University, Japan)

**Abstract :** In this paper, we present the first linear delay algorithms to enumerate all 2-edge-connected induced subgraphs and to enumerate all 2-vertex-connected induced subgraphs for a given simple undirected graph. We treat these subgraph enumeration problems in a more general framework based on set systems. For an element set  $V$ ,  $(V, \mathcal{C} \subseteq 2^V)$  is called a {em set system}, where we call  $C \in \mathcal{C}$  a {em component}. A nonempty subset  $Y \subseteq C$  is a {em removable set of  $C$ } if  $C \setminus Y$  is a component and  $Y$  is a {em minimal removable set} ({em MRS}) {em of  $C$ } if it is a removable set and no proper nonempty subset  $Z \subsetneq Y$  is a removable set of  $C$ . We say that a set system has {em subset-disjoint} ({em SD}) property if, for every two components  $C, C' \in \mathcal{C}$  with  $C' \not\subseteq C$ , every MRS  $Y$  of  $C$  satisfies either  $Y \subseteq C'$  or  $Y \cap C' = \emptyset$ . We assume that a set system with SD property is implicitly given by an oracle that returns an MRS of a component which is given as a query. We provide an algorithm that, given a component  $C$ , enumerates all components that are subsets of  $C$  in linear time/space with respect to  $|V|$  and oracle running time/space. We then show that, given a simple undirected graph  $G$ , the pair of the vertex set  $V = V(G)$  and the family of vertex subsets that induce 2-edge-connected (or 2-vertex-connected) subgraphs of  $G$  has SD property, where an MRS in a 2-edge-connected (or 2-vertex-connected) induced subgraph corresponds to either an ear or a single vertex with degree greater than two.

## [00626] Finite element complexes for structure-preservation in continuum mechanics

**Session Time & Room :**

00626 (1/3) : 2E (Aug.22, 17:40-19:20) @E710

00626 (2/3) : 3C (Aug.23, 13:20-15:00) @E710

00626 (3/3) : 3D (Aug.23, 15:30-17:10) @E710

**Type :** Proposal of Minisymposium

**Abstract :** Exact sequences of function spaces, called complexes, have played a central role in developing structure-preserving numerical methods in the framework of the finite element exterior calculus. Discrete preservation of the underlying complex structure between function spaces often preserves physical quantities and conservation laws of interest; examples include pressure-robust schemes for Navier-Stokes flows, conservation of angular momentum in linear elasticity, and propagation of the constraint equations of general relativity. In this minisymposium, we seek to investigate how far this approach can be taken by bringing together numerical analysts from across the broad spectrum of continuum mechanics problems arising in applications.

**Organizer(s) :** Francis Aznaran, Charles Parker

**Classification :** 65N30, 65N12, 74S05

**Minisymposium Program :**

00626 (1/3) : 2E @E710 [Chair: Charles Parker]

## [02976] Finite element gradgrad and divdiv complexes in three dimensions

**Format :** Talk at Waseda University

**Author(s) :** Jun Hu (Peking University)Yizhou Liang (University of Augsburg)Rui Ma (Beijing Institute of Technology)

**Abstract :** We introduce the first family of conforming discrete gradgrad complexes and divdiv complexes in three dimensions. In gradgrad complexes, the first construction of finite element spaces of  $H(\text{curl}, \mathbb{S})$  and  $H(\text{div}, \mathbb{T})$  was proposed, and in divdiv complexes , finite element spaces of  $H(\text{sym curl}, \mathbb{T})$  are newly constructed. We prove that these finite element complexes are exact. We also present a special family of degrees of freedom of these complexes.

## [05087] Structure-preserving discretization for wave equations

**Format :** Talk at Waseda University

**Author(s) :** Sanna Mönkölä (University of Jyväskylä)Jonni Lohi (University of Jyväskylä)Markus Kivioja (University of Jyväskylä)Tytti Saksa (University of Jyväskylä)Lauri Kettunen (University of Jyväskylä)Tuomo Rossi (University of Jyväskylä)

**Abstract :** We present a comprehensive framework for linear wave equations to consider hyperbolic problems in both classical and quantum mechanics. The framework is based on differential geometry in  $(d+1)$ -dimensional spacetime. To discretize the equations, we use a spacetime extension of the discrete exterior calculus including a leapfrog-style evolution in the time direction. To demonstrate the efficacy of this approach, we carry out numerical simulations using a C++ software library developed at the University of Jyväskylä.

## [03866] Regge finite elements and the linearized Einstein tensor

**Format :** Talk at Waseda University

**Author(s) :** Evan Gawlik (University of Hawaii)Michael Neunteufel (TU Wien)

**Abstract :** In general relativity, the linearization of the Einstein tensor plays an important role in studies of gravitational waves. We study the action of this differential operator on elements of the Regge finite element space: piecewise polynomial symmetric (0,2)-tensor fields with tangential-tangential continuity across simplex interfaces. We show that the Regge finite elements and the linearized Einstein operator fit into a commutative diagram of differential complexes that generalizes one studied by Christiansen in the lowest-order setting.

## [03058] Variational structures in cochain projection based discretization of classical field theories

**Format :** Talk at Waseda University

**Author(s) :** Brian Tran (UC San Diego)Melvin Leok (UC San Diego)

**Abstract :** Compatible discretizations, such as finite element exterior calculus, provide a discretization framework that respect the cohomological structure of the de Rham complex, which can be used to systematically construct stable mixed finite element methods. Multisymplectic variational integrators are a class of geometric numerical integrators for Lagrangian and Hamiltonian field theories, and they yield methods that preserve the multisymplectic structure and momentum-conservation properties of the continuous system. In this talk, we discuss the synthesis of these two approaches, by constructing discretization of the variational principle for Lagrangian field theories utilizing structure-preserving finite element projections. In our investigation, compatible discretization by cochain projections plays a pivotal role in the preservation of the variational structure at the discrete level, allowing the discrete variational structure to essentially be the restriction of the continuum variational structure to a finite-dimensional subspace. The preservation of the variational structure at the discrete level will allow us to construct a discrete Cartan form, which encodes the variational structure of the discrete theory, and subsequently, we utilize the discrete Cartan form to naturally state discrete analogues of Noether's theorem and multisymplecticity. Time permitting, we will relate the covariant spacetime discretization to the tensor product discretization approach using variational integration in space and symplectic integration in time.

00626 (2/3) : 3C @E710 [Chair: Francis Aznaran]

## [02047] Local Exactness of de Rham Conforming Hierarchical B-spline Differential Forms

**Format :** Talk at Waseda University

**Author(s) :** Kendrick M Shepherd (Brigham Young University)Deepesh Toshniwal (TU Delft)

**Abstract :** Conservation laws present in partial differential equations arising in fluid mechanics and electromagnetics are frequently described using the de Rham sequence of differential forms. Stability of numerical methods solving these equations requires discrete preservation of these conservation laws. This talk will present sufficient local exactness criteria for a set of smooth, high-order, isogeometric, locally-refinable spline spaces in Euclidean space of arbitrary dimension in order to enable stable high-order, geometrically-precise finite element analyses.

## [02065] Multigrid solvers for the de Rham complex with optimal complexity in polynomial degree

**Format :** Talk at Waseda University

**Author(s) :** Pablo D. Brubeck (University of Oxford)Patrick Emmet Farrell (University of Oxford)

**Abstract :** We present multigrid solvers for the high-order FEM de Rham complex with the same time and space complexity as sum-factorized operator application. Our approach relies on new finite elements with orthogonality properties on the reference hexahedron. The resulting sparsity enables the fast solution of the patch problems arising in the Pavarino, Arnold–Falk–Winther, and Hiptmair space decompositions, in the separable case. In the non-separable case, the method can be applied to a sparse auxiliary operator.

## [04622] On partially continuous finite element spaces in variational problems of continuum mechanics

**Format :** Talk at Waseda University

**Author(s) :** Adam Sky (University of Luxembourg)

**Abstract :** The use of partially continuous finite element spaces in continuum mechanics is well-established. Common applications are mixed formulations, for example in linear elasticity. While strongly symmetric finite elements for the discretisation of the stresses have been introduced, their mapping from a reference element is non-trivial. As such, in the first part of this talk we will introduce simple mappings for base functions of the Hu-Zhang element, which are applicable to hp-FEM, and discuss related problems in linear elasticity.

Linear elasticity represents one limited model of continuum mechanics. With the goal of describing more complex phenomena, generalised continua have been introduced. In the context of the linear relaxed micromorphic model, the strain field is augmented via a microdistortion field. In recent works, it was proven that the field can be defined in  $H(\text{symCurl})$ , such that well-posedness is maintained. With that in mind, the second part of this talk will discuss novel finite elements for the discretisation of the  $H(\text{symCurl})$ -space and their application to the relaxed micromorphic sequence.

## [05396] New Class of Stabilized Mixed FEM for Compressible and Incompressible Nonlinear Elasticity

**Format :** Talk at Waseda University

**Author(s) :** Ali Gerami Matin (The George Washington University)

**Abstract :** In this paper, we introduce two stabilized class of mixed finite element methods with bubble functions and a perturbation method for 2D and 3D compressible and incompressible nonlinear elasticity. Two approaches, namely, the  $L^2$ -projection and projections of partly sobolev classes, have been employed to obtain weak formulations. Both structured and unstructured simplicial meshes have been considered to investigate effects of different meshes on our formulation. Finally, by solving some benchmark problems, we investigate performance of the stabilized elements in different circumstances. Benchmark results demonstrate that our stabilized formulation provide a robust and computationally efficient way of simulating compressible, near-incompressible, and incompressible materials. These formulations also show good performance in approximating stress and pressure in bending problems, 2D and 3D solids with complex geometries, and heterogeneous bodies.

00626 (3/3) : 3D @E710 [Chair: Francis Aznaran]

## [05491] Machine-Learned Whitney Forms for Structure Preservation

**Format :** Talk at Waseda University

**Author(s) :** Jonas Albert Actor (Sandia National Laboratories)Nathaniel Trask (Sandia National Laboratories)Andy Huang (Sandia National Laboratories)

**Abstract :** For many applications, scientific machine learning techniques provide few guarantees on structure preservation or convergence rates. Towards this limitation, we introduce a partition of unity architecture to parameterize data-driven Whitney forms, allowing discovery of mixed finite element spaces. The resulting geometric parameterization extracts reduced models from full-field data while exactly preserving physics and matching expected convergence rates. We provide examples for  $H(\text{div})$  problems in two dimensions, highlighting the capabilities of the learned Whitney form architecture.

## [04438] Study of a structure preserving discretization framework for Maxwell-Klein-Gordon equations.

**Format :** Online Talk on Zoom

**Author(s) :** Snorre Christiansen (University of Oslo)Tore Halvorsen (University of Oslo)Claire Scheid (Côte d'Azur University)

**Abstract :** We propose a numerical discretization framework for a general family of gauge invariant mechanical Lagrangian. Through the definition of a discrete gauge invariant Lagrangian, we study a fully discrete leap-frog time integration scheme based on conforming space discretizations. We prove the stability and convergence of the scheme without the a priori knowledge of the solution. We will then show how our general framework apply to the Maxwell-Klein-Gordon system.

## [05131] Compatible finite elements for terrain following meshes

**Format :** Talk at Waseda University

**Author(s) :** Karina Kowalczyk (Imperial College London)Colin J Cotter (Imperial College London)

**Abstract :** In this talk we are presenting a new approach for compatible finite element discretisations for atmospheric flows on a terrain following mesh. In classical compatible finite element discretisations, the  $H(\text{div})$ -velocity space involves the application of Piola transforms when mapping from a reference element to the physical element in order to guarantee normal continuity. In the case of a terrain following mesh, this causes an undesired coupling of the horizontal and vertical velocity components. We are proposing a new finite element space, that drops the Piola transform. For solving the equations we introduce a hybridisable formulation with trace variables supported on horizontal cell faces in order to enforce the normal continuity of the velocity in the solution. Alongside the discrete formulation for various fluid equations we discuss solver and time-stepping approaches that are compatible with them and present our latest numerical results. In the case of the Helmholtz equations we give a proof of well-posedness of the arising discrete system.

## [04775] Structure-preserving discretization of momentum-based formulations of fluids using discrete exterior calculus

**Format :** Talk at Waseda University

**Author(s) :** Christopher Eldred (Sandia National Laboratories)

**Abstract :** Representation of physical quantities as differential forms (using exterior calculus) has proved to be a powerful approach to formulating continuum mechanics. However, most prior work has focused on scalar-valued differential forms, and therefore electrodynamics and velocity-based formulations of fluids. This talk will present progress towards a discrete exterior calculus for (vector) bundle-valued differential forms, such as those needed to describe momentum, and illustrate its applicability for discretization of momentum-based formulations of (charged) fluid models.

# [00632] From model-blind to model-aware learning of inverse problems in imaging

**Session Time & Room :**

00632 (1/2) : 3C (Aug.23, 13:20-15:00) @E812

00632 (2/2) : 3D (Aug.23, 15:30-17:10) @E812

**Type :** Proposal of Minisymposium

**Abstract :** In recent years, there has been an increasing interest in exploring how to combine the practical advantages of learning-based methods with the theoretical understanding and the convergence guarantees coming from model-based approaches for the regularisation of ill-posed inverse problems. This mini-symposium will bring together researchers working on data-driven methods and deep learning for inverse problems in the attempt to providing an overview of the mathematical insights able to shed light on how learned image reconstruction approaches can be reliable tools for real-world applications.

**Organizer(s) :** Tatiana A. Bubba, Luca Calatroni, Luca Ratti

**Classification :** 68T07, 65R32, 45Q05, artificial neural networks, deep learning, inverse problems

**Minisymposium Program :**

## [03849] Untrained networks with latent-space disentanglement for motion separation in videos

**Format :** Talk at Waseda University

**Author(s) :** Malena Sabaté Landman (Department of Applied Mathematics and Theoretical Physics, University of Cambridge)Abudllah Abudllah (Department of Mathematics, The Chinese University of Hong Kong)Martin Holler (Institute of Mathematics and Scientific Computing, University of Graz)Karl Kunisch (Institute of Mathematics and Scientific Computing, University of Graz)

**Abstract :** In this talk I will present an algorithm that allows to efficiently isolate different, highly non-linear motion types in video data, using untrained generator networks together with a specific technique for latent space disentanglement that uses minimal, one-dimensional information on some of the underlying dynamics.

## [01569] Continuous Generative Neural Networks for Inverse Problems

**Format :** Talk at Waseda University

**Author(s) :** Giovanni Alberti (University of Genoa)Matteo Santacesaria (University of Genoa)Silvia Sciuotto (University of Genoa)

**Abstract :** We study Continuous Generative Neural Networks CGNNs, namely, generative models in the continuous setting. The architecture is inspired by DCGAN, with one fully connected layer, several convolutional layers and nonlinear activation functions. In the continuous  $L^2$  setting, the dimensions of the spaces of each layer are replaced by the scales of a multiresolution analysis of a compactly supported wavelet. We present conditions on the convolutional filters and on the nonlinearity that guarantee that a CGNN is injective. This theory finds applications to inverse problems, and allows for deriving Lipschitz stability estimates for possibly nonlinear infinite-dimensional inverse problems with unknowns belonging to the manifold generated by a CGNN.

## [02780] Learned proximal operators in accelerated unfolded methods with pseudodifferential operators

**Format :** Online Talk on Zoom

**Author(s) :** Andrea Sebastiani (University of Bologna)Tatiana Alessandra Bubba (University of Bath)Luca Ratti (University of Genoa)Subhadip Mukherjee (University of Bath)

**Abstract :** In recent years, hybrid reconstruction frameworks have been proposed by unfolding iterative methods and learning a suitable pseudodifferential correction on the part that can provably not be handled by model-based methods. In this talk, I will present a variant of this approach, where an accelerated iterative algorithm is unfolded and the proximal operator is replaced by learned operators, as in the PnP framework. The numerical experiments on limited-angle CT achieve promising results.

## [02946] Electrical impedance tomography, virtual X-rays, and stroke

**Format :** Talk at Waseda University

**Author(s) :** Samuli Siltanen (University of Helsinki)

**Abstract :** A connection between Electrical Impedance Tomography (EIT) and X-ray tomography was found in (Greenleaf et al. 2018) using microlocal analysis. Fourier transform applied to the spectral parameter of Complex Geometric Optics solutions produces virtual X-ray projections, enabling a novel filtered back-projection type nonlinear reconstruction algorithm for EIT. This approach is called Virtual Hybrid Edge Detection. Machine learning can be used for classifying stroke (into ischemic and hemorrhagic) based on virtual X-ray profiles of the conductivity.

00632 (2/2) : 3D @E812 [Chair: Luca Ratti]

## [03308] Beyond supervised learning in imaging: measurement-driven computational imaging

**Format :** Talk at Waseda University

**Author(s) :** Julian Tachella (CNRS, ENSL)

**Abstract :** Most computational imaging algorithms rely either on hand-crafted prior models (total variation, wavelets) or on supervised learning with a ground truth dataset of references. The first approach generally obtains suboptimal reconstructions, whereas the latter is impractical in many scientific and medical imaging applications where ground-truth data is expensive or even impossible to obtain. In this talk, I will present recent algorithmic and theoretical advances in unsupervised learning for imaging inverse problems that overcome these limitations, by learning from noisy and incomplete measurement data alone and leveraging weak prior knowledge on the reconstructed image distribution, such as invariance to groups of transformations (rotations, translations, etc.) and low-dimensionality.

## [03519] Deep Learning for Reconstruction in Nano CT

**Format :** Talk at Waseda University

**Author(s) :** Alice Oberacker (Saarland University)Anne Wald (Georg-August-Universität Göttingen)Bernadette Hahn-Rigaud (Universität Stuttgart)Tobias Kluth (Universität Bremen)Johannes Leuschner (Universität Bremen)Maximilian Schmidt (Universität Bremen)Thomas Schuster (Saarland University)

**Abstract :** Tomographic X-ray imaging at the nano-scale helps reveal the structures of materials like alloys and biological tissue. However, environmental perturbances during data acquisition can cause motion between the object and scanner. To reduce noise in the back-projection, a learned version of the RESESOP-Kaczmarz method was investigated. The deep network was trained with simulated imaging data to unroll the iterative reconstruction process, allowing the network to learn the back-projected image after a fixed number of iterations.

## [04062] Learning intrinsic shape representations via LBO spectra

**Format :** Talk at Waseda University

**Author(s) :** serena morigi (University of Bologna)

**Abstract :** Neural fields are emerging as a new function representation paradigm for image processing, computer vision, computer graphics, and more. The intrinsic neural fields rely on a feature embedding based on the Laplace Beltrami Operator. We derive the embedding functions from the solution of graph Laplacian-based variational regularization problems. This allows to impose property which directly derived from the associated variational formulation. An efficient model-aware method as well as a model-blind neural network will be presented.

## [04272] Inexact Algorithms for Bilevel Learning

**Format :** Talk at Waseda University

**Author(s) :** Mohammad Sadegh Salehi (University of Bath)

**Abstract :** We consider hyperparameter estimation for variational methods formulated as a bilevel learning problem. Due to the use of numerical solvers, one can only compute an inexact gradient with respect to the hyperparameters. We introduce and analyse a new framework that dynamically updates the accuracy in inexact algorithms and selects stepsizes based on linesearch. We compare the performance of our method with existing methods through numerical experiments.

# [00633] Unconventional numerical methods for advection-diffusion PDEs

**Session Time & Room :**

00633 (1/2) : 4E (Aug,24, 17:40-19:20) @E705

00633 (2/2) : 5B (Aug,25, 10:40-12:20) @E705

**Type :** Proposal of Minisymposium

**Abstract :** Advection-diffusion PDEs represent a broad range of mathematical models in different fields of science and engineering, involving physical processes such as fluid flow, heat and mass transfer, diffusion, etc. Discretizations of advection-diffusion PDEs must be physically consistent, accurate and efficient on emerging computing architectures. The purpose of this minisymposium is to showcase recent developments in numerical methods that explore unconventional approaches to address these challenges. Methods such as residual distribution, flux-corrected transport, hybridized DG and FEM, SBP-SAT, machine learning enhanced methods, as well as methods for non-local extensions of classical advection-diffusion PDEs are of particular interest to this minisymposium.

**Organizer(s) :** Svetlana Tokareva, Nathaniel Morgan, Dmitri Kuzmin, Remi Abgrall

**Classification :** 65Mxx

**Minisymposium Program :**

00633 (1/2) : 4E @E705 [Chair: Steven Walton]

## [03915] Dissipation-based WENO stabilization of high-order finite element methods for hyperbolic problems

**Format :** Online Talk on Zoom

**Author(s) :** Dmitri Kuzmin (TU Dortmund University)Joshua Vedral (TU Dortmund University)

**Abstract :** We propose a new kind of weighted essentially nonoscillatory (WENO) schemes to high-order finite element discretizations of hyperbolic conservation laws. In contrast to WENO-based limiters for DG approximations, our approach uses a reconstruction-based smoothness sensor to blend the numerical viscosity operators of high- and low-order stabilization terms. The so-defined hybrid approximation introduces low-order nonlinear diffusion in the vicinity of shocks, while preserving the high-order accuracy of the baseline discretization in regions where the exact solution is smooth. The underlying reconstruction procedure performs Hermite interpolation on stencils consisting of a mesh cell and its neighbors. The amount of numerical dissipation depends on the relative differences between partial derivatives of reconstructed candidate polynomials and those of the consistent finite element approximation. All derivatives are taken into account by the employed smoothness sensor. To assess the accuracy of our WENO scheme, we derive error estimates and perform numerical experiments. In particular, we prove that the consistency error of the nonlinear stabilization is of the order  $p+1/2$ , where  $p$  is the polynomial degree. For uniform meshes and smooth exact solutions, the experimentally observed rate of convergence is as high as  $p+1$ .

## [04012] A Residual Distribution Approach to Isotropic Wave Kinetic Equations

**Format :** Talk at Waseda University

**Author(s) :** Steven Walton (Los Alamos National Laboratory)

**Abstract :** We present a Petrov-Galerkin Residual Distribution (PG-RD) approach to solve isotropic wave kinetic equations (WKEs). The RD method is well-known for its ability to accurately solve advection dominated flow problems due to its intrinsic multi-dimensional upwinding property. While WKEs are nonlinear and non-local integro-differential equations, very different from the historical applications of RD methods, the energy flux of the equations we consider is local. We show that the PG-RD method derived generalizes a finite volume scheme given in a previous work. Analysis of the convergence properties of the method is also provided. The method is verified against established theoretical work for isotropic WKEs.

## [04019] High order Flux Reconstruction schemes for turbulent flows and spectral analysis

**Format :** Talk at Waseda University

**Author(s) :** ROMARIC SIMO TAMOU (IFPEN)JULIEN BOHBOT (IFPEN)JULIEN COATLÉVEN (IFPEN)VINCENT PERRIER (INRIA)QUANG HUY TRAN (IFPEN)

**Abstract :** This study focuses on evaluating Flux Reconstruction schemes for turbulent flows. For these schemes, we perform new analyses of their dissipation and dispersion properties, and we find consistent results with the classical analysis. Ultimately, we evaluate the effect of the high order and correction functions on the DNS of Taylor-Green vortex. This work provides valuable insights into the performance of FR schemes for turbulent flows and presents a promising new approach for analyzing their stability.

## [04429] The Cartesian Grid Active Flux Method with Adaptive Mesh Refinement

**Format :** Talk at Waseda University

**Author(s) :** Erik Chudzik Christiane Helzel (Heinrich-Heine Universität)

**Abstract :** We present the first implementation of the Active Flux method on Cartesian grids with adaptive mesh refinement: A new finite volume method for hyperbolic conservation laws, that was introduced by Eymann and Roe, which uses a continuous, piecewise quadratic reconstruction and Simpson's rule to compute numerical fluxes. Point values at grid cell interfaces together with cell averages are used to compute the reconstruction. The resulting method is third order accurate and has a compact stencil in space and time.

00633 (2/2) : 5B @E705 [Chair: Eric Tovar]

## [04883] Optimization-based, property-preserving algorithm for passive tracer transport

**Format :** Talk at Waseda University

**Author(s) :** Pavel Bochev (Sandia National Laboratories)Kara Peterson (Sandia National Laboratories)Denis Ridzal (Sandia National Laboratories)

**Abstract :** We present a new optimization-based property-preserving algorithm for passive tracer transport. The algorithm utilizes a semi-Lagrangian approach based on incremental remapping of the mass and the total tracer.

part\_1

However, unlike traditional semi-Lagrangian schemes, which remap the density and the tracer mixing ratio through monotone reconstruction or flux correction, we utilize an optimization-based remapping that enforces conservation and local bounds as optimization constraints.

In so doing we separate accuracy considerations from preservation of physical properties to obtain a conservative, second-order accurate transport scheme that also has a notion of optimality. Moreover, we prove that the optimization-based algorithm preserves linear relationships between tracer mixing ratios. We illustrate the properties of the new algorithm using a series of standard tracer transport test problems in a plane and on a sphere.

## **[04980] Multi-material ALE remap: interface sharpening in a matrix-free computation**

**Format :** Talk at Waseda University

**Author(s) :** Vladimir Z Tomov (Lawrence Livermore National Lab)Tzanio Kolev (Lawrence Livermore National Laboratory)Robert Rieben (Lawrence Livermore National Lab)Arturo Vargas (Lawrence Livermore National Lab)

**Abstract :** We propose a new method for remap of material volume fractions, densities, and specific internal energies in the context of compressible ALE hydrodynamics. The remap is based on advection in pseudotime. As the volume fraction method can diffuse materials over many mesh elements, we introduce a sharpening modification on PDE level. We explain the effects of the modification and how it produces results that are still conservative and bounded. The latter involves FCT-type methods. The second major contribution, next to sharpening, is that all remap methods avoid assembly of global matrices. This avoids data motion and provides higher computational efficiency.

Performed under the auspices of the U.S. Department of Energy under Contract DE-AC52-07NA27344 (LLNL-ABS-847808)

## **[05104] Robust second-order approximation of the compressible Euler Equations with an arbitrary equation of state**

**Format :** Talk at Waseda University

**Author(s) :** Eric Joseph Tovar (Los Alamos National Laboratory)Bennett Clayton (Texas A&M University)Jean-Luc Guermond (Texas A&M University)Matthias Maier (Texas A&M University)Bojan Popov (Texas A&M University)

**Abstract :** This work is concerned with constructing a robust, high-order approximation of the compressible Euler equations for gas dynamics supplemented with an arbitrary or tabulated equation of state. In particular, we show how to construct a high-order graph-viscosity coefficient using an interpolated entropy pair useful when the equation of state is given by tabulated experimental data. Similarly, we construct an entropy surrogate functional that is used in a convex limiting technique that preserves the invariant domain of the system. Finally, the numerical method is then verified with analytical solutions and then validated with several benchmarks seen in the literature and laboratory experiments.

## **[05153] Heuristic Topological Estimation of Reduced Order Model Basis Functions from PDE Solution Snapshots**

**Format :** Talk at Waseda University

**Author(s) :** Candace Pauline Diaz (Sandia National Laboratories)Pavel Bochev (Sandia National Laboratories)Denis Ridzal (Sandia National Laboratories)

**Abstract :** Proper Orthogonal Decomposition (POD) is a common approach to obtain reduced basis sets for projection-based model reduction. For some classes of problems, such as hyperbolic Partial Differential Equations (PDEs), POD does not always achieve reasonable order reduction due to the lack of exponential decay of the leading singular values. In this work we investigate persistent homology as an alternative approach for deriving reduced order basis functions that may be particularly parsimonious for such PDEs.

## **[00635] Mean field games and optimal transport with applications in data science and biology**

**Session Time & Room :**

00635 (1/2) : 1C (Aug.21, 13:20-15:00) @F403

00635 (2/2) : 1D (Aug.21, 15:30-17:10) @F403

**Type :** Proposal of Minisymposium

**Abstract :** Mean field games (MFG) study the behavior of individual players in large populations, where each player controls their own state, while some collective behavior is considered for decision-making. Specific MFG models can be formulated as generalized measure transportation problems, exemplifying one of the tight connections to optimal transport (OT).

This mini-symposium highlights the close relationship between MFG and OT, advancing research directions in modeling and numerical algorithms, and expanding fields of applications. Particular emphasis will lie on new applications in data science, such as point-cloud analysis on networks, and in biology, such as single-cell data integration.

**Organizer(s) :** Shiying Li, Wuchen Li, Siting Liu, Caroline Moosmueller

**Classification :** 49N80, 49N90, 68T09, 92-10

**Minisymposium Program :**

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00635 (1/2) : 1C @F403 [Chair: Caroline Moosmueller]

## [05205] Manifold Interpolating Optimal-Transport Flows for Trajectory Inference

**Format :** Online Talk on Zoom

**Author(s) :** Smita Krishnaswamy (Yale University)Guillaume Huguet (University of Montreal)Alexander Tong (University of Montreal )Oluwadamilola Fasina (Yale University)Daniel Sumner Magruder (Yale University)Manik Kuchroo (Yale University)Guy Wolf (University of Montreal)

**Abstract :** We present a method called Manifold Interpolating Optimal-Transport Flow (MIOFlow) that learns stochastic, continuous population dynamics from static snapshot samples taken at sporadic timepoints. MIOFlow combines dynamic models, manifold learning, and optimal transport by training neural ordinary differential equations (Neural ODE) to interpolate between static population snapshots as penalized by optimal transport with manifold ground distance. Further, we ensure that the flow follows the geometry by operating in the latent space of an autoencoder that we call a geodesic autoencoder (GAE). In GAE the latent space distance between points is regularized to match a novel multiscale geodesic distance on the data manifold that we define. We show that this method is superior to normalizing flows, Schrödinger bridges and other generative models that are designed to flow from noise to data in terms of interpolating between populations. Theoretically, we link these trajectories with dynamic optimal transport. We evaluate our method on simulated data with bifurcations and merges, as well as scRNA-seq data from embryoid body differentiation, and acute myeloid leukemia treatment.

## [01462] A Distributed Algorithm for Wasserstein Proximal Operator Splitting

**Format :** Online Talk on Zoom

**Author(s) :** Iman Nodouzi (University of California Santa Cruz)Abhishek Halder (University of California Santa Cruz)

**Abstract :** Many time-stepping algorithms are available to numerically realize the Wasserstein proximal updates, which generalize the concept of gradient steps to the manifold of probability measures. This talk will present a distributed algorithm to perform the Wasserstein proximal updates. The proposed algorithm generalizes the finite dimensional Euclidean consensus ADMM to the measure-valued Wasserstein, and to its entropy-regularized version. We will explain how the proposed algorithm differs compared to the Euclidean case, and will provide numerical case-studies.

## [05216] Wasserstein gradient flows and Hamiltonian flows on the generative model

**Format :** Online Talk on Zoom

**Author(s) :** Shu Liu (Math department, UCLA)Wuchen Li (University of South Carolina)Hao Wu (Georgia Institute of Technology)Xiaojing Ye (Georgia State University)Haomin Zhou (Georgia Institute of Technology)

**Abstract :** In this talk, we introduce a series of sampling-friendly, optimization-free methods for computing high-dimensional gradient flows and Hamiltonian flows on the Wasserstein probability manifold by leveraging generative models from deep learning. Such methods project the corresponding probability flows to parameter space and obtain finite-dimensional ordinary differential equations (ODEs) which can be directly solved by using classical numerical methods. Furthermore, the computed generative models can efficiently generate samples from the probability flows via pushforward maps.

## [05393] Linear Optimal Transport (LOT) Framework for Graph-Based Semi-Supervised Learning using Point Cloud Data

**Format :** Talk at Waseda University

**Author(s) :** Mary Chriselda Antony Oliver (University of Cambridge) Michael Roberts (University of Cambridge) Matthew Thorpe (University of Manchester)

**Abstract :** In this study, we introduce a novel application of the linear optimal transport (LOT) framework, leveraging the geometrical structure of its linear embeddings. We incorporate these embeddings in the form of projections (velocity fields) post dimensionality reduction using graph-based semi-supervised algorithms. Additionally, we compute the shortest path between two prominent nodes (geodesic) for the feature vector within the graphical setting. Finally, we demonstrate the performance through numerical experiments conducted on benchmark 3-D point cloud data.

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00635 (2/2) : 1D @F403 [Chair: Wuchen Li]

## [05294] Towards a mathematical theory of development

**Format :** Talk at Waseda University

**Author(s) :** Geoffrey Schiebinger (University of British Columbia)

**Abstract :** This talk introduces a mathematical theory of developmental biology, based on optimal transport. While, in principle, organisms are made of molecules whose motions are described by the Schrödinger equation, there are simply too many molecules for this to be useful. Optimal transport provides a set of equations that describe development at the level of cells. We propose that this optimal transport hypothesis is a fundamental mathematical principle of developmental biology.

## [03712] Applications of Gromov-Wasserstein Distance to Graph and Hypergraph Analysis

**Format :** Talk at Waseda University

**Author(s) :** Tom Needham (Florida State University)

**Abstract :** Gromov-Wasserstein distances are metrics, inspired by the usual Wasserstein distances of optimal transport, which are designed to handle comparisons between distributions that lie on different spaces. I will overview some recent applications of these metrics to the analysis of graph and hypergraph datasets.

## [03382] Single-cell data integration using optimal transport

**Format :** Talk at Waseda University

**Author(s) :** Ritambhara Singh (Brown University) Pinar Demetci (Brown University) Rebecca Santorella (Brown University) Bjorn Sandstede (Brown University) William Stafford Noble (University of Washington) Ievgen Redko (Jean Monet University, Saint Etienne) Quang Huy Tran (Université Bretagne-Sud, CNRS, IRISA, Vannes)

**Abstract :** Integration of single-cell multi-omic measurements is crucial to understand the underlying biology. However, this is particularly challenging due to the lack of sample-wise or feature-wise correspondence information across single-cell datasets generated from different samples. In this talk, I will present our optimal transport-based integration methods that perform the alignment of different single-cell measurements with minimal supervision. We demonstrate their state-of-the-art performance on simulations and real-world datasets.

## [03962] Multi-agent reinforcement learning for collaborative games: a mean-field perspective

**Format :** Online Talk on Zoom

**Author(s) :** Haotian Gu (UC Berkeley) Xin Guo (UC Berkeley) Renyuan Xu (University of Southern California) Xiaoli Wei (Tsinghua-Berkeley Institute)

**Abstract :** Multi-agent reinforcement learning (MARL) has enjoyed substantial successes in many applications including real-time resource allocation, order matching for ride-hailing, and autonomous driving. Despite the empirical success of MARL, general theories behind MARL algorithms are less developed due to the intractability of interactions, complex information structure, and the curse of dimensionality. Instead of directly analyzing the multi-agent systems, the mean-field theory provides a powerful approach to approximate the games under various notions of equilibria. Moreover, the analytically feasible framework of mean-field theory leads to efficient and tractable learning algorithms with theoretical guarantees.

In this talk, we will demonstrate how mean-field theory can contribute to analyzing a class of simultaneous-learning-and-decision-making problems under cooperation, with unknown rewards and dynamics. Moreover, we will show that the learning procedure can be further decentralized and scaled up if a network structure is specified. Our result lays the first theoretical foundation for the so-called "centralized training and decentralized execution" scheme, a widely used training scheme in the empirical works of cooperative MARL problems.

# [00638] Minisymposium on Interaction between Harmonic Analysis and Data Science

## **Session Time & Room :**

00638 (1/3) : 3E (Aug.23, 17:40-19:20) @E812

00638 (2/3) : 4C (Aug.24, 13:20-15:00) @E812

00638 (3/3) : 4D (Aug.24, 15:30-17:10) @E812

## **Type :** Proposal of Minisymposium

**Abstract :** Over the last twenty years, data science, machine learning, and deep learning in particular, has begun transforming the global economy and modern life. While much attention is focused on purely empirical data mining results, there are considerable mathematical structures and a growing body of theory about how the structures relate to observable properties of real-world systems. Discovering such structures may lead to important mathematical insights and implications for practitioners. The minisymposium will facilitate interactions between harmonic analysts and experts on the theory of data science, machine learning, and deep learning to foster further research in this fast developing area.

**Organizer(s) :** Hrushikesh Mhaskar, Nicole Muecke, Ding-Xuan Zhou

**Classification :** 68T07, 41A63, 42C40, 68Q32

## **Minisymposium Program :**

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00638 (1/3) : 3E @E812 [Chair: Dingxuan Zhou]

## **[01801] Algorithms for quantizing neural networks with guaranteed accuracy**

### **Format :** Talk at Waseda University

**Author(s) :** Rayan Saab (University of California San Diego)

**Abstract :** We present both deterministic and stochastic algorithms for quantizing neural networks, which can achieve significant savings in cost, computation time, memory, and power consumption while preserving the network's performance. Our methods are data-driven, computationally efficient, and have provable error guarantees. We showcase our results through numerical experiments on large multi-layer networks. Time permitting, we also discuss open problems and connections to other areas of research. This is joint work, in parts, with Jinjie Zhang, Yixuan Zhou, and Johannes Maly.

## **[01538] Learning nonlinear functionals using deep ReLU networks**

### **Format :** Talk at Waseda University

**Author(s) :** Linhao Song (City University of Hong Kong)Jun Fan (Hong Kong Baptist University)Dingxuan Zhou (University of Sydney)

**Abstract :** Functional neural networks have been proposed and studied in order to approximate nonlinear continuous functionals defined on  $L^p([-1, 1]^s)$  for integers  $s \geq 1$  and  $1 \leq p < \infty$ . However, their theoretical properties are largely unknown beyond universality of approximation or the existing analysis does not apply to the rectified linear unit (ReLU) activation function. In this talk we investigate the approximation power of functional deep ReLU networks and establish their rates of approximation under mild regularity conditions.

## **[01578] Compressed sensing for the sparse Radon transform**

### **Format :** Talk at Waseda University

**Author(s) :** Giovanni S. Alberti (University of Genoa)Matteo Santacesaria (University of Genoa)S. Ivan Trapasso (Polytechnic University of Turin)Alessandro Felisi (University of Genoa)

**Abstract :** Compressed sensing allows for the recovery of signals from a number of measurements that is proportional, up to logarithmic factors, to their sparsity. The classical theory considers random linear measurements or subsampled isometries, with applications to, e.g., MRI. I will show how compressed sensing can be applied to the sparse Radon transform, where a finite number of angles are considered. The result follows from a new theory of compressed sensing for infinite-dimensional ill-posed problems.

**[01808] Super-resolution of sparse measures: recent advances****Format :** Online Talk on Zoom**Author(s) :** Dmitry Batenkov (Tel Aviv University)**Abstract :** The problem of sparse super-resolution asks to recover a linear combination of Dirac point measures from low-frequency and inaccurate measurements. This is a popular model for applications including spectral estimation, direction of arrival, imaging of point sources, and sampling of signals below the Nyquist limit.

In this talk I will describe recent results on deriving optimal recovery bounds and corresponding algorithms for this model and its generalizations to sparse distributions defined on homogeneous Riemannian manifolds.

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00638 (2/3) : 4C @E812 [Chair: Hrushikesh Mhaskar]

**[04107] Proximal neural networks and Plug-and-Play methods****Format :** Talk at Waseda University**Author(s) :** Gabriele Steidl (TU Berlin) Johannes Hertrich (TU Berlin) Sebastian Jonas Neumayer (EPFL)**Abstract :** We introduce stable tight frame proximal neural networks (PNNs)

which are by construction averaged operators.

For the training of PNNs, we propose a stochastic gradient descent on (a submanifold of) the Stiefel manifold.

First, we apply cPNN based denoisers within a Plug-and-Play framework and provide convergence results for the corresponding PnP forward-backward splitting algorithm based on an oracle construction.

Second, we use the averagedness property of PNNs to construct a new architecture within residual flows.

**[03587] The Bayesian Learning Rule****Format :** Talk at Waseda University**Author(s) :** Mohammad Emtiyaz Khan (RIKEN Center for AIP)**Abstract :** Humans and animals have a natural ability to autonomously learn and quickly adapt to their surroundings. How can we design machines that do the same? In this talk, I will present Bayesian principles to bridge such gaps between humans and machines. I will show that a wide-variety of machine-learning algorithms are instances of a single learning-rule derived from Bayesian principles. The rule unravels a dual perspective yielding new mechanisms for knowledge transfer in learning machines. My hope is to convince the audience that Bayesian principles are indispensable for an AI that learns as efficiently as we do.**[02888] Learning linear operators: Infinite-dimensional regression as a well-behaved non-compact inverse problem****Format :** Talk at Waseda University**Author(s) :** Nicole Mücke (TU Brunswick)**Abstract :** We consider the problem of learning a linear operator between two Hilbert spaces from empirical observations, which we interpret as least squares regression in infinite dimensions. We show that this goal can be reformulated as an inverse problem with the feature that its forward operator is generally non-compact.

We prove that this inverse problem is equivalent to the known compact inverse problem associated with scalar response regression.

Our framework allows for obtaining dimension-free rates for generic learning algorithms. They hold for a variety of practically-relevant scenarios in functional regression as well as nonlinear regression with operator-valued kernels and match those of classical kernel regression with scalar response.

**[02915] A Non-Asymptotic Analysis of Dropout in the Linear Model****Format :** Talk at Waseda University**Author(s) :** Gabriel Clara (University of Twente) Sophie Langer (University of Twente) Johannes Schmidt-Hieber (University of Twente)**Abstract :** We investigate the statistical behavior of iterates generated by gradient descent with dropout in a linear model. Non-asymptotic convergence rates for expectations and covariance matrices of the iterates are presented. Difficulties arising from the interaction between gradient descent dynamics and the variance added by dropout are examined. The results motivate and support discussion of statistical aspects of dropout, focusing on optimality of the variance.

00638 (3/3) : 4D @E812 [Chair: Nicole Mücke]

## [04309] Direct method for function approximation on data defined manifolds, II

**Format :** Talk at Waseda University

**Author(s) :** Hrushikesh Mhaskar (Claremont Graduate University) Ryan Michael O'Dowd (Claremont Graduate University)

**Abstract :** In theoretical analysis of function approximation in the context of machine learning, a standard approach is to assume that given data lies on an unknown manifold. We view the unknown manifold as a sub-manifold of an ambient hypersphere and construct a one-shot approximation using spherical polynomials. Our approach does not require pre-processing of the data to obtain information about the manifold other than its dimension. We give optimal rates of approximation for relatively "rough" functions.

## [04364] Distribution learning for count data

**Format :** Talk at Waseda University

**Author(s) :** Xin Guo (The University of Queensland) Qiang Fu (The University of British Columbia) Tian-Yi Zhou (Georgia Institute of Technology) Hien Nguyen (The University of Queensland)

**Abstract :** Parameter and density estimation for count models are classical problems in statistics, and are widely used in many branches of physical and social sciences. Grouped and right-censored (GRC) counts are widely used in criminology, demography, epidemiology, marketing, sociology, psychology and other related disciplines to study behavioural and event frequencies, especially when sensitive research topics or individuals with possibly lower cognitive capacities are at stake. Yet, the co-existence of grouping and right-censoring poses major difficulties in regression analysis. To implement generalised linear regression of GRC counts, we derive modified Poisson estimators and their asymptotic properties, develop a hybrid line search algorithm for parameter inference, demonstrate the finite-sample performance of these estimators via simulation, and evaluate its empirical applicability based on survey data of drug use in America. This method has a clear methodological advantage over the ordered logistic model for analysing GRC counts. We will also present our recent works on mixing density estimation through kernel methods and deep neural networks.

## [05188] Hierarchical systems of exponential bases for partitions of intervals

**Format :** Online Talk on Zoom

**Author(s) :** Goetz Pfander (Catholic University Eichstätt Ingolstadt, Mathematical Institute for Machine Learning and Data Science) David Walnut (George Mason University)

**Abstract :** Fourier series form a cornerstone of analysis; it allows the expansion of a complex valued 1-periodic function in the basis of integer frequency exponentials. A simple rescaling argument shows that by splitting the integers into evens and odds, we obtain orthogonal bases for functions defined on the first, respectively the second half of the unit interval. We develop generalizations of this curiosity and show that, for example, for any finite partition of the unit interval into subintervals exists a partition of integers into subsets, each of which forms a basis for functions supported on the respective subinterval.

## [00639] Analytical and computational aspects of topological photonics

**Session Time & Room :**

00639 (1/2) : 4E (Aug.24, 17:40-19:20) @E710

00639 (2/2) : 5B (Aug.25, 10:40-12:20) @E710

**Type :** Proposal of Minisymposium

**Abstract :** Topological photonics is an emerging area in material sciences that explores and utilizes the topological invariants of photonic materials, which take integer values and are robust against system disorder. The area has attracted significant interest in recent years due to the ability of topological photonic materials to transport photon energy in a very robust manner, yet its mathematical development is in its infancy. This minisymposium aims to bring together mathematicians and scientists interested in this interdisciplinary area to share recent results and exchange ideas.

**Organizer(s) :** Chiu-Yen Kao, Junshan Lin, Braxton Osting

**Classification :** 35P05, 35B10, 35Q93, 49R05, 65K10

**Minisymposium Program :**

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00639 (1/2) : 4E @E710 [Chair: Braxton Osting]

## [03761] TE band structure of high contrast honeycomb photonic crystals

**Format :** Talk at Waseda University

**Author(s) :** Maxence Cassier (Aix Marseille Univ, CNRS, Centrale Marseille, Institut Fresnel, Marseille, France)Michael Weinstein (Dept of Applied Physics & Applied Mathematics, and Dept. of Mathematics, Columbia University, New-York, United States)

**Abstract :** We analyse the propagation of transverse electric (TE) waves in a two dimensional honeycomb photonic medium.

This medium consists of a homogeneous bulk of fixed permittivity and an array of high permittivity dielectric inclusions centered at the vertices of a honeycomb lattice. Our mathematical results, supported by numerical simulations, give detailed local information about the conical crossings of dispersion surfaces (Dirac points) as well as global information about the high contrast behavior of dispersion surfaces.

## [03902] Super band gaps and interface modes in one-dimensional quasicrystals

**Format :** Talk at Waseda University

**Author(s) :** Bryn Davies (Imperial College London)Lorenzo Morini (Cardiff University)Richard Craster (Imperial College London)

**Abstract :** Quasicrystalline photonic crystals show significant potential (large spectral gaps and robustness) but are underutilised in applications due to the lack of efficient modelling techniques. In this work, we show that periodic (supercell) approximations give accurate predictions of the main spectral gaps of Fibonacci quasicrystals. This is based on characterising the growth of the underlying recursion relation and corroborates the existence of previously observed “super band gaps”. We also present a strategy for creating interface modes.

## [03872] Mathematical theory for the interface mode in a waveguide bifurcated from a Dirac point

**Format :** Talk at Waseda University

**Author(s) :** Jiayu QIU (Hong Kong University of Science and Technology)Junshan LIN (Auburn University)Peng XIE (Hong Kong University of Science and Technology)Hai ZHANG (Hong Kong University of Science and Technology)

**Abstract :** In this talk, we present our new results on the existence of a bound state in a waveguide consisting of two semi-infinite periodic structures separated by an interface. The two periodic structures are perturbed from the same periodic medium with a Dirac point, and possess a common band gap enclosing the Dirac point. Using the layer potential technique and asymptotic analysis, we are able to overcome the difficulty imposed by the sharp interface.

## [05154] Bloch Waves for Maxwell's Equations in High-Contrast Photonic Crystals

**Format :** Talk at Waseda University

**Author(s) :** Robert Paul Viator (Swarthmore College)Robert Lipton (Louisiana State University)Silvia Jimenez Bolanos (Colgate University)Abiti Adili (University of Massachusetts - Lowell)

**Abstract :** We investigate the Bloch spectrum of a 3-dimensional high-contrast photonic crystal. The Bloch eigenvalues, for fixed quasi-momentum, are expanded in a power series in the material contrast parameter in the high-contrast limit, together with a convergence radius, obtained by decomposing an appropriate vectorial Sobolev space into three mutually orthogonal curl-free subspaces. We also identify the limit spectrum in the periodic case. Time permitting, we will describe some geometries which admit this spectral structure.

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00639 (2/2) : 5B @E710 [Chair: Chiu-Yen Kao]

## [05207] Pseudo-magnetism and Landau Levels in strained 2-dimensional photonic crystals

**Format :** Online Talk on Zoom

**Author(s) :** Michael I Weinstein (Columbia University)

**Abstract :** The principal use of photonic crystals is to engineer the photonic density of states, which controls light-matter coupling. We show theoretically that a strained 2D honeycomb photonic crystal can generate artificial electromagnetic fields and highly degenerate Landau

levels, having high density of states. Since the tight-binding approximation is generally not applicable to photonics, we employ a multiscale analysis

of the full continuum 2D Helmholtz wave equation and derive effective Dirac equations with pseudo-magnetic and pseudo-electric potentials for the dynamics of wave-packets. The deformation can be chosen to induce a constant pseudo-magnetic field, for which the effective Hamiltonian has Landau level spectrum.

Our numerical simulations of the full continuum wave equations show mildly dispersive Landau levels, which we show can be “flattened” by adjusting the pseudo-electric potential.

This theory is joint work with J. Guglielmon and M.C. Rechtsman.

The predictions have recently been corroborated in optical experiments, in joint work with M. Barsukova, Z. Zhang, B. Zhen, L. He, F. Grisé, R. McEntaffer, S. Vaidya, J. Guglielmon and M.C. Rechtsman

## [05298] Quantized Fractional Thouless Pumping of Solitons

**Format :** Online Talk on Zoom

**Author(s) :** Mikael Rechtsman (Penn State Univ)

**Abstract :** I will present my group’s recent work on the fractional pumping of solitons in photonic Thouless pumps. Specifically, I will show that the displacement (in unit cells) of solitons in Thouless pumps is strictly quantized to the Chern number of the band from which the soliton bifurcates in the low power regime; whereas in the intermediate power regime, nonlinear bifurcations lead to fractional quantization of soliton motion. This fractional quantization can be predicted from multi-band Wannier functions associated with the states of the pump.

## [04812] Topological insulators in semiclassical regime

**Format :** Online Talk on Zoom

**Author(s) :** Alexis Drouot (University of Washington)

**Abstract :** I will study a semiclassical Dirac equation that originates in the field of topological insulators. The semiclassical regime allows to make sense of propagating and counter-propagating companion states. We’ll derive speed and profile for wavepackets corresponding to topological edge states, and show that the counter-propagating state disperses strongly -- an unusual phenomena in the analysis of coherent states.

## [05311] Topological-cavity surface-emitting laser

**Format :** Online Talk on Zoom

**Author(s) :** Ling Lu (Institute of Physics, CAS)

**Abstract :** Contrary to the perception that the Nobel-winning topological physics has not found useful applications, we show that the textbook design of daily-life semiconductor lasers are equivalent to standard topological models in 1D. By upgrading to the 2D vortex zero mode, we invent the topological-cavity surface-emitting lasers (TCSEL) whose performance far exceeds that of the commercial counterparts. Finally, we demonstrate the monopole cavity in 3D with the optimal single-mode behavior, completing the kink-vortex-monopole trilogy of topological defect modes.

# [00640] Variational Analysis: Theory and Applications

**Session Time & Room :**

00640 (1/2) : 2C (Aug.22, 13:20-15:00) @F401

00640 (2/2) : 2D (Aug.22, 15:30-17:10) @F401

**Type :** Proposal of Minisymposium

**Abstract :** Variational Analysis lies at the heart of modern optimization and underlies the convergence analysis of many algorithms. The purpose of this session is to bring together selected experts from the worldwide optimization and analysis communities to exchange ideas and present new results. We will strike a balance between early-career researchers and experts.

**Organizer(s) :** Heinz Bauschke, Xianfu Wang

**Classification :** 49J53, 65K10, 90C25, Variational Analysis, Convex Analysis and Optimization Methods

**Minisymposium Program :**

00640 (1/2) : 2C @F401 [Chair: Shawn Xianfu Wang]

## [01802] Fixed point strategies for sparsity aware inverse problems and hierarchical convex optimization

**Format :** Talk at Waseda University

**Author(s) :** Isao Yamada (Tokyo Institute of Technology)Masao Yamagishi (Tokyo Institute of Technology)

**Abstract :** We present central ideas behind the recently developed fixed point strategies for a nonconvexly regularized sparse least squares model and a hierarchical convex optimization problem. Related advancements for nonconvex optimization and signal processing will also be introduced briefly.

## [02724] The splitting algorithms by Ryu, by Malitsky-Tam, and by Campoy applied to normal cones of linear subspaces converge strongly to the projection onto the intersection

**Format :** Talk at Waseda University

**Author(s) :** Heinz H Bauschke (University of British Columbia Okanagan)Shambhavi Singh (University of British Columbia Okanagan)shawn xianfu wang (University of British Columbia Okanagan)

**Abstract :** Finding a zero of a sum of maximally monotone operators is a fundamental problem in modern optimization and nonsmooth analysis. Assuming that the resolvents of the operators are available, this problem can be tackled with the Douglas-Rachford algorithm. However, when dealing with three or more operators, one must work in a product space with as many factors as there are operators. In groundbreaking recent work by Ryu and by Malitsky and Tam, it was shown that the number of factors can be reduced by one. A similar reduction was achieved recently by Campoy through a clever reformulation originally proposed by Kruger. All three splitting methods guarantee weak convergence to some solution of the underlying sum problem; strong convergence holds in the presence of uniform monotonicity.

In this paper, we provide a case study when the operators involved are normal cone operators of subspaces and the solution set is thus the intersection of the subspaces. Even though these operators lack strict convexity, we show that striking conclusions are available in this case: strong (instead of weak) convergence and the solution obtained is (not arbitrary but) the projection onto the intersection. Numerical experiments to illustrate our results are also provided.

## [02977] Fixed Point Algorithms: Convergence, stability and data dependence results

**Format :** Talk at Waseda University

**Author(s) :** Javid Ali (Aligarh Muslim University, Aligarh)

**Abstract :** {\\bf Abstract.} In this talk, we discuss a newly introduced two step fixed point iterative algorithm. We prove a strong convergence result for weak contractions. We also prove stability and data dependency of a proposed iterative algorithm. Furthermore, we utilize our main result to approximate the solution of a nonlinear functional Volterra integral equation. Some numerical examples are also furnished. If time permits, then we will discuss Image recovery problem as well.

00640 (2/2) : 2D @F401 [Chair: Shawn Xianfu Wang]

## [01896] Adaptive proximal algorithms for convex optimization under local Lipschitz continuity of the gradient

**Format :** Talk at Waseda University

**Author(s) :** Puya Latafat (KU Leuven)Andreas Themelis (Kyushu University)Lorenzo Stella (Amazon Berlin)Panagiotis Patrinos (KU Leuven)

**Abstract :** Gradient-based proximal algorithms have traditionally been bound to global Lipschitz differentiability requirements. Attempts to widen their applicability or reduce conservatism typically involve wasteful trial-and-error backtracking routines. Extending recent advancements in the smooth setting, we show how for convex problems it is possible to avoid backtrackings altogether and retrieve stepsizes adaptively without function evaluations. We demonstrate this with an adaptive primal-dual three-term splitting method that includes proximal gradient as special case.

## [02427] Level proximal subdifferential and its resolvent

**Format :** Talk at Waseda University

**Author(s) :** Ziyuan Wang (University of British Columbia)shawn xianfu wang (University of British Columbia)

**Abstract :** In this talk, we introduce a new subdifferential whose resolvent completely represents the associated proximal operator. After illustrating that the usual limiting subdifferential representation is only valid when the given function is weakly convex, we propose level proximal subdifferential, which is a careful refinement of the well-known proximal subdifferential. As such, its resolvent always coincides with the associated proximal operator regardless of weak

convexity. Besides this pleasant identity, we also investigate several useful properties of level proximal subdifferential. Finally, numerous examples are given to further illustrate our results.

### [02993] On quasidifferentiability and optimization problems

**Format :** Talk at Waseda University

**Author(s) :** VIVEK LAHA (Banaras Hindu University)

**Abstract :** The talk presents suitable optimality conditions based on some recent works in fractional programming and variational inequalities in terms of quasidifferentials. The presentation deals with Fritz-John and Karush-Kuhn-Tucker type necessary optimality conditions at an optimal point in the framework of the quasidifferentiable analysis. Further, several other applications of the results are investigated in different fields of optimization like mathematical programs with equilibrium constraints and/or vanishing constraints.

## [00641] Emerging Collaborations: Mathematical Views of Modelling Biological Scales

**Session Time & Room :**

00641 (1/2) : 1C (Aug.21, 13:20-15:00) @A512

00641 (2/2) : 1D (Aug.21, 15:30-17:10) @A512

**Type :** Proposal of Minisymposium

**Abstract :** In this session, we highlight interdisciplinary efforts of mathematicians whose work integrates biological processes and mathematical tools. Often researchers focus on modeling or simulating with a particular biological scale in mind while neglecting the dynamical connections across scales. The aims of the work showcased in this symposium are to develop and use efficient algorithms, data structures, visualization, and communication tools with the goal of computer modeling of biological systems from the cellular to the population scale. This minisymposium features speakers who are currently working in this area and have an interest in establishing new collaborations.

**Organizer(s) :** Amy Buchmann, Candice Price, Arietta Fleming-Davies

**Classification :** 92-10, 92-08, 92Cxx, 92Dxx, Mathematical Modelling, Systems Biology, Computational Biology

**Minisymposium Program :**

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00641 (1/2) : 1C @A512 [Chair: Amy Buchmann]

### [01865] A Multiscale, Interdisciplinary Approach to Blood Clot Degradation

**Format :** Talk at Waseda University

**Author(s) :** Brittany Bannish (University of Central Oklahoma)Nathan Hudson (East Carolina University)Valerie Tutwiler (Rutgers University)

**Abstract :** Blood clots are critical to prevent bleeding, but complications arise when clots are not degraded effectively. We present a stochastic model of clot degradation that includes structural and biochemical details from the single fiber to full clot scales. We show that modeling in tandem with laboratory experimentation yields physiological insights that were impossible with models or experiments alone. We also discuss the need for future models that include mechanical forces.

### [01970] Explorations of DNA Knot Shadows

**Format :** Talk at Waseda University

**Author(s) :** Candice Price (Smith College)

**Abstract :** A core question in knot theory is: How do we identify whether two knots are equivalent under a specific set of operations? Knot theory deals not only with the curious variations in the underlying topological structure, e.g. strands, loops, choice of operations of knots, but also with invariants, e.g. Alexander, Jones, link homologies. Knot theory has been used in various fields of mathematics and has become an essential resource for understanding the topology and the geometry of DNA. In this presentation, we will describe and explore our work to interpret 2-dimensional projections of knots, called knot shadows.

## [02104] A mathematical approach to understanding reproductive health disparities at the intersection of ovulatory and metabolic dysfunction

**Format :** Talk at Waseda University

**Author(s) :** Erica J Graham (Bryn Mawr College)

**Abstract :** Endocrine physiology is a complex system of crosstalk between hormones in various tissues. Reproductive hormone dysregulation may disrupt ovulation and may be exacerbated by metabolic abnormalities. Racial and ethnic disparities are also prevalent at the intersection of metabolic and ovarian dysfunction. Here we introduce a mathematical model of the human ovulatory cycle and consider mechanisms of disruption to characterize ovulatory phenotypes. We then examine how health disparities might influence--or be influenced by--model-based phenotypes.

## [02133] Harmonic Analysis on Simplicial Simplexes: How far could we take it?

**Format :** Talk at Waseda University

**Author(s) :** Karamatou Yacoubou Djima (Wellesley College)

**Abstract :** Networks' emergence as an ideal setting for studying complex systems brought enormous interest in extending powerful harmonic analysis (HA) tools from Euclidean spaces to graphs. Most efforts focused on the graph Laplacian's eigendecomposition, producing results such as the graph Fourier transform. Recently, the same endeavor moved to higher-order network structures—simplicial simplexes. We survey classical Fourier analysis and its graph extensions before presenting new developments and challenges of HA on simplicial complexes based on the Hodge Laplacian.

00641 (2/2) : 1D @A512 [Chair: Candice Price]

## [02145] Ecological consequences of heterogeneity in host-pathogen population dynamics

**Format :** Talk at Waseda University

**Author(s) :** Arietta Fleming-Davies (University of San Diego)

**Abstract :** Variation within-species is key in evolutionary processes. We asked how quantitative variation changes along with mean differences in pathogen performance across populations of the hosts they infect. We fit statistical models incorporating a Gamma distribution of host disease susceptibility to experimental dose response data from an insect baculovirus system, to ask how variation in infectivity might change with genotype by genotype ( $G \times G$ ) combinations of pathogen and host populations.

## [02146] Modeling microscale biofluids

**Format :** Talk at Waseda University

**Author(s) :** Amy Lyn Buchmann (University of San Diego)

**Abstract :** Mathematical models can be used to study the role of hydrodynamic interactions in the coordination and self-organization of microorganisms. For example, cilia self-organize to form a metachronal wave that propels the surrounding fluid, yet how this organization occurs is not well understood. Additionally, the coordination of bacterial flagella may be studied to inspire the development of motors in microfluidic devices that can effectively mix and pump a viscous fluid. Here we present a mathematical model to study the interactions between elastic structures in a viscous fluid and investigate their coordination.

## [02152] We are what we eat: a mathematical model of the gut-brain axis.

**Format :** Talk at Waseda University

**Author(s) :** Ami Radunskaya (Pomona College)

**Abstract :** The “gut-brain axis” is the communication between the enteric nervous system (in the gut) and the central nervous system (in the brain). Over the past few decades, scientists have collected data that confirms a bidirectional communication channel between these two nervous systems that is closely tied to the bacterial ecology of the gut, the production of serotonin in both the gut and the brain, and the interaction of serotonin with other hormones. We propose a mathematical model that illuminates both the dynamics of this communication channel and the effect of perturbations due to treatment strategies.

## [02213] Modeling the long term effects of thermoregulation on human sleep

**Format :** Talk at Waseda University

**Author(s) :** Alicia Prieto Langarica (Youngstown State University)

**Abstract :** The connection between human sleep and energy exertion has long been regarded as part of the reasoning for the need to sleep. We used to think that we sleep in order to rest. However, a recent theory proposes a different

explanation, one that unifies sleep among all species. This talk presents a mathematical model of human sleep/wake regulation with thermoregulatory functions. The model is used to gain quantitative insight into the effects of ambient temperature on sleep quality and how this relates to the unifying theory for sleep.

## [00642] Traveling Waves in Mathematical Epidemiology

**Session Time & Room :** 1C (Aug.21, 13:20-15:00) @G601

**Type :** Proposal of Minisymposium

**Abstract :** Wave propagation in epidemic models is known as one of the interesting issues in the field of mathematical epidemiology. Mathematical theory of traveling wave solutions in epidemic models has been developed in recent years. In many cases, the basic reproduction number or a corresponding threshold value plays an important role in determining the existence of the traveling wave. The purpose of this minisymposium is to share and discuss recent developments and results on this topic among interested researchers.

**Organizer(s) :** Yoichi Enatsu, Toshikazu Kuniya

**Classification :** 35C07, 35K57, 92D30

**Minisymposium Program :**

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00642 (1/1) : 1C @G601 [Chair: Toshikazu Kuniya]

### [05106] Traveling wave solutions for an epidemic model with free boundary

**Format :** Talk at Waseda University

**Author(s) :** Yoichi Enatsu (Tokyo University of Science)Emiko Ishiwata (Tokyo University of Science)Takeo Ushijima (Tokyo University of Science)

**Abstract :** Free boundary problems are recently used to model phenomena of biological invasion for species such as migration into a new habitat. In this talk, we consider a diffusive epidemic model with free boundary. We prove the existence and nonexistence of a traveling wave solution of the model. We numerically observe the traveling wave and the front motion of the model. This is a joint work with Takeo Ushijima and Emiko Ishiwata.

### [01447] Traveling Wave Solutions for Discrete Diffusive SIR Epidemic Model

**Format :** Talk at Waseda University

**Author(s) :** Ran Zhang (Heilongjiang University)Jinliang Wang (Heilongjiang University)Shengqiang Liu (Tiangong University)

**Abstract :** In this talk, we deal with the conditions of existence and nonexistence of traveling wave solutions for a class of discrete diffusive epidemic model. In addition, the boundary asymptotic behavior of traveling wave solutions is obtained by constructing a suitable Lyapunov functional and employing Lebesgue dominated convergence theorem. Our result could answer some unsolved problems in the previous studies on discrete diffusive epidemic model.

### [04496] Traveling waves of a differential-difference diffusive Kermack-McKendrick epidemic model with age-structured protection phase

**Format :** Talk at Waseda University

**Author(s) :** Mostafa Adimy (Inria and UCBL 1, Lyon)Abdennasser Chekroun (University of Tlemcen)Toshikazu Kuniya (Kobe University)

**Abstract :** We consider a general class of diffusive Kermack-McKendrick SIR epidemic models with an age-structured protection phase with limited duration, for example due to vaccination or drugs with temporary immunity. A saturated incidence rate is also considered which is more realistic than the bilinear rate. The characteristics method reduces the model to a coupled system of a reaction-diffusion equation and a continuous difference equation with a time-delay and a nonlocal spatial term caused by individuals moving during their protection phase. We study the existence and non-existence of non-trivial traveling wave solutions. We get almost complete information on the threshold and the minimal wave speed that describes the transition between the existence and non-existence of non-trivial traveling waves that indicate whether the epidemic can spread or not. We discuss how model parameters, such as protection rates, affect the minimal wave speed. The difficulty of our model is to combine a reaction-diffusion system with a continuous difference equation. We deal with our problem mainly by using Schauder's fixed point theorem. More precisely, we reduce the problem of the existence of non-trivial traveling wave solutions to the existence of an admissible pair of upper and lower solutions.

## [00643] Stochastic modeling in cell biology

**Session Time & Room :**

00643 (1/3) : 1E (Aug.21, 17:40-19:20) @A512

00643 (2/3) : 2C (Aug.22, 13:20-15:00) @A512

00643 (3/3) : 2D (Aug.22, 15:30-17:10) @A512

**Type :** Proposal of Minisymposium

**Abstract :** Emerging forms of experimental data in cellular and molecular biology have driven new modeling frameworks, many of which are stochastic due to noisy characteristics at these scales. This session features stochastic model construction and analysis of microbiological systems ranging in scale from the movement of genetic material (e.g., DNA) to multi-cell tissues, including mathematical advances motivated by the challenges to explain observed phenomena. Mathematical themes will include stochastic differential equations, Monte Carlo techniques for stochastic simulation, and stochastic PDEs. Several talks will also incorporate novel approaches to effectively representing and incorporating experimental data into the modeling process.

**Organizer(s) :** Peter Kramer, Christopher Miles

**Classification :** 92-10, 60G07, 35Q92, 62M30

**Minisymposium Program :**


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00643 (1/3) : 1E @A512 [Chair: Peter Kramer]

## [04558] Intracellular Transport Across Scales

**Format :** Talk at Waseda University

**Author(s) :** Keisha Cook (Clemson University)Scott A. McKinley (Tulane University)

**Abstract :** Biological systems are traditionally studied as isolated processes (e.g. regulatory pathways, motor protein dynamics, transport of organelles, etc.). Although more recent approaches have been developed to study whole cell dynamics, integrating knowledge across biological levels remains largely unexplored. In experimental processes, we assume that the state of the system is unknown until we sample it. Many scales are necessary to quantify the dynamics of different processes. These may include a magnitude of measurements, multiple detection intensities, or variation in the magnitude of observations. The interconnection between scales, where events happening at one scale are directly influencing events occurring at other scales, can be accomplished using mathematical tools for integration to connect and predict complex biological outcomes. In this work we focus on building inference methods to study the complexity of the cytoskeleton from one scale to another.

## [02757] Inferring RNA Dynamic Rates from Spatial Stochastic Snapshots

**Format :** Talk at Waseda University

**Author(s) :** Christopher Edward Miles (University of California, Irvine)

**Abstract :** There are unresolved mysteries about the dynamics of RNA splicing, an important molecular process in the genetic machinery. These mysteries remain because the obtainable data for this process are not time series, but rather static spatial images of cells with stochastic particles. From a modeling perspective, this creates a challenge of finding the right mathematical description that respects the stochasticity of individual particles but remains computationally tractable. I'll share our approach to constructing a spatial Cox process with intensity governed by a reaction-diffusion PDE. We can do inference on this process with experimental images by employing variational Bayesian inference. Several outstanding issues remain about how to combine classical and modern statistical/data-science approaches with more exotic mechanistic models in biology. This work is in collaboration with the Ding lab of Biomedical Engineering at UCI.

## [02952] Centrosome Movement and Clustering During Mitosis

**Format :** Online Talk on Zoom

**Author(s) :** Sarah Olson (Worcester Polytechnic Institute)Amity Manning (Worcester Polytechnic Institute)

**Abstract :** While much work has been done to understand the roles of the key molecular components of the mitotic spindle

during cell division, identifying the consequences of force perturbations in the spindle remains a challenge. In particular, cells with extra centrosomes may undergo a bipolar or multipolar division. We combine experimental approaches with computational modeling to define a role for cortical dynein in centrosome clustering, allowing for a bipolar division in cells with extra centrosomes.

**[01821] Stochastic model of nuclear size control in *S. pombe*****Format :** Online Talk on Zoom**Author(s) :** Xuesong Bai (Brandeis University)Thomas Fai (Brandeis University)**Abstract :** The size of the nucleus scales robustly with cell size so that the nuclear-to-cell size—the N/C ratio—is maintained during growth in many cell types. To address the fundamental question of how cells maintain the size of their organelles despite the constant turnover of proteins and biomolecules, we consider a model based on osmotic force balance predicts a stable nuclear-to-cell size ratio, in good agreement with experiments on the fission yeast *Schizosaccharomyces pombe*. We model the synthesis of macromolecules during growth using chemical kinetics and demonstrate how the N/C ratio is maintained in homeostasis. We compare the variance in the N/C ratio predicted by the model to that observed experimentally.

00643 (2/3) : 2C @A512 [Chair: Christopher Miles]

**[05399] Stochastic models of DNA methylation, plasticity and drug resistance****Format :** Online Talk on Zoom**Author(s) :** Jasmine Foo (University of Minnesota)**Abstract :** In this talk I will discuss some recent work on modeling stochastic intracellular DNA methylation processes and examine their consequences on population dynamics within a growing tumor.**[04460] Stochastic modeling of ovarian aging****Format :** Online Talk on Zoom**Author(s) :** Sean Lawley (University of Utah)**Abstract :** Why are women born with up to a million primordial follicles when only a few hundred will ever ovulate a mature egg? What physiological mechanisms trigger menopause? Can the age of natural menopause be predicted? Can menopause be delayed? In this talk, we will describe recent stochastic models of ovarian aging which are aimed at answering these questions.

00643 (3/3) : 2D @A512 [Chair: Christopher Miles]

**[02211] Optimal curvature and directional sensing in long-range cell-cell communication****Format :** Talk at Waseda University**Author(s) :** Jun Allard (University of California Irvine)Sohyeon Park (University of California Irvine)Dae Seok Eom (University of California Irvine)Hyunjoong Kim (University of Pennsylvania)**Abstract :** Cells in tissue can communicate long-range via diffusive signals. In addition, another class of cell-cell communication is by long, thin cellular protrusions that are  $\sim 100$  microns in length, i.e., many cell-lengths, and  $\sim 100$  nanometers in width, i.e., below traditional microscope resolution. These protrusions have been recently discovered in many organisms, including nanotubes humans and airinemes in zebrafish. But, before establishing communication, these protrusions must find their target cell. Here we demonstrate airinemes in zebrafish are consistent with a finite persistent random walk model. We study this model by stochastic simulation, and by numerically solving the survival probability equation using Strang splitting. The probability of contacting the target cell is maximized for a balance between ballistic search and diffusive highly curved, random search. We find that the curvature of airinemes in zebrafish, extracted from live cell microscopy, is approximately the same value as the optimum in the simple persistent random walk model. We also explore the ability of the target cell to infer direction of the airineme's source, finding the experimentally observed parameters to be at a Pareto optimum balancing directional sensing with contact initiation.**[04467] Centrosome asymmetry in the early *C. elegans* embryo****Format :** Talk at Waseda University**Author(s) :** Adriana Dawes (Ohio State University)Shayne Plourde (The Ohio State University)David Ignacio (The Ohio State University)Andrew Cohen (The Ohio State University)**Abstract :** Centrosome positioning, which determines where a cell divides, is mediated by microtubules, biopolymers nucleated at the centrosomes, and the motor protein dynein. Using stochastic and continuum models along with a measure of centrosome movement, we identify key proteins involved in regulating centrosome movement in early embryos of the nematode worm *C. elegans*, and demonstrate the parallel role of cell geometry in proper positioning of the centrosomes.

## [04462] Modeling and tracking random motion in micrometer-scale living systems

**Format :** Talk at Waseda University

**Author(s) :** Jay Mack Newby (University of Alberta)

**Abstract :** We study stochastic motion of objects in micrometer-scale living systems: tracer particles in living cells, pathogens in mucus, and single cells foraging for food. We use stochastic models and state space models to track objects through time and infer properties of objects and their surroundings. For example, we can calculate the distribution of first passage times for a pathogen to cross a mucus barrier, or we can spatially resolve the fluid properties of the cytoplasm in a living cell. Recently developed computational tools, particularly in the area of Markov Chain Monte Carlo, are creating new opportunities to improve multiple object tracking. The primary remaining challenge, called the data association problem, involves mapping measurement data (e.g., positions of objects in a video) to objects through time. I will discuss new developments in the field and ongoing efforts in my lab to implement them. I will motivate these techniques with specific examples that include tracking salmonella in GI mucus, genetically expressed proteins in the cell cytoplasm, active transport of nuclei in multinucleate fungal cells, and raphid diatoms in seawater surface interfaces.

## [04071] Stochastic effects in molecular motor teams under detachment and reattachment

**Format :** Talk at Waseda University

**Author(s) :** Peter Kramer (Rensselaer Polytechnic Institute)Joseph Klobusicky (The University of Scranton)John Fricks (Arizona State University)

**Abstract :** We revisit two paradigms of cooperative action by kinesin molecular motors involving a coupling of the detachment and reattachment processes with the stochastic spatial dynamics. First, for two dissimilar types of kinesin transporting a common cargo, we provide approximate analytical characterizations for how incorporating slack in the tether model affects the cooperative dynamics. Secondly, we extend consideration of gliding assays to a situation where microtubules are crosslinked while being crowdsurfed by immobilized kinesin.

## [00652] Recent Advances in Quasi-Monte Carlo Methods and Related Topics

**Session Time & Room :**

00652 (1/3) : 5B (Aug.25, 10:40-12:20) @G304

00652 (2/3) : 5C (Aug.25, 13:20-15:00) @G304

00652 (3/3) : 5D (Aug.25, 15:30-17:10) @G304

**Type :** Proposal of Minisymposium

**Abstract :** Many applications, such as computational finance, uncertainty quantification involving PDEs with random inputs, and training of deep neural networks, require tackling computational problems with high dimensions. This minisymposium will bring together people working in Quasi-Monte Carlo (QMC) methods, a powerful class of methods for such problems with high dimensionality. More specifically, QMC methods have been proved efficient for integration over the multi-dimensional unit cube, over other domains, function approximation, and density estimation. In this minisymposium, we aim to showcase recent advances in QMC methods and foster interaction between researchers working in these areas.

**Organizer(s) :** Takashi Goda, Yoshihito Kazashi

**Classification :** 11K45, 41A55, 65C05, 65D30, 65D32

**Minisymposium Program :**

00652 (1/3) : 5B @G304 [Chair: Takashi Goda]

## [04989] The fast reduced QMC matrix-vector product

**Format :** Talk at Waseda University

**Author(s) :** Josef Dick (UNSW)Adrian Ebert (JKU Linz)Lukas Herrmann (RICAM Linz)Peter Kritzer (RICAM Linz)Marcello Longo (ETH Zurich)

**Abstract :** We study the approximation of integrals of the form  $\int_D f(\mathbf{x}^\top A) d\mu(\mathbf{x})$ , where  $A$  is a matrix, by quasi-Monte Carlo (QMC) rules  $N^{-1} \sum_{k=0}^{N-1} f(\mathbf{x}_k^\top A)$ . We are interested in cases where the main computational cost in computing the

approximation arises from the computation of  $\mathbf{x}_k^\top A$ . We design QMC rules for which the computation of  $\mathbf{x}_k^\top A$ ,  $k = 0, 1, \dots, N - 1$  can be done in a fast way.

## [05066] Recent Advances on discrepancy and WCE of constructible point sets on spheres

**Format :** Talk at Waseda University

**Author(s) :** Johann S. Brauchart (Graz University of Technology)

**Abstract :** We discuss bounds for the  $L_2$ -discrepancy and worst-case error for equal-weight quasi Monte Carlo rules (and compare them with optimal bounds) for constructible  $N$ -point sets that arise from mapping rational lattice points in the plane to the sphere using an area preserving Lambert transformation. Our standard examples are spherical Fibonacci point configurations defined by a Fibonacci lattice in the unit square.

This is joint work with Josef Dick (UNSW) and Yuan Xu (University of Oregon).

## [03448] Quasi-Monte Carlo approach to Bayesian optimal experimental design

**Format :** Talk at Waseda University

**Author(s) :** Vesa Kaarnioja (Free University of Berlin)

**Abstract :** The goal in Bayesian optimal experimental design (OED) is to maximize the expected information gain for the reconstruction of unknown quantities given a limited budget for collecting measurement data. Quasi-Monte Carlo (QMC) methods have been demonstrated to be effective for numerical treatment of partial differential equations (PDEs) involving input uncertainties in recent years. In this talk, we derive tailored QMC cubature rules to reduce the computational burden in Bayesian OED problems governed by PDEs.

## [04877] Density estimation by Monte Carlo and quasi-Monte Carlo

**Format :** Talk at Waseda University

**Author(s) :** Pierre L'Ecuyer (University of Montreal)

**Abstract :** Estimating the density of a continuous random variable  $X$  has been studied extensively in settings where  $n$  independent observations of  $X$  are given a priori. Popular methods include histograms and kernel density estimators. These methods have bias and their mean square error converges at a slower rate than the usual  $O(1/n)$  rate. In this talk, we consider the situation where the observations are generated by Monte Carlo simulation from a model. Unbiased estimators and better convergence rates can then be obtained, sometimes much better than  $O(1/n)$ . We show how this can be achieved, using techniques such as conditional Monte Carlo, likelihood ratio methods for derivative estimation, and randomized quasi-Monte Carlo. Theoretical and empirical results will be given. This is based on joint work with Amal Ben Abdellah and Florian Puchhammer.

00652 (2/3) : 5C @G304 [Chair: Yoshihito Kazashi]

## [03343] High dimensional approximation and the curse of dimensionality

**Format :** Talk at Waseda University

**Author(s) :** Ian Hugh Sloan (UNSW Sydney)

**Abstract :** This talk, joint work with Kuo and Kaarnioja, extends a 2022 result with Kazashi and Nobile. It uses periodic kernels located at lattice points. The lattice points and the kernels depend on parameters called “weights”. Using new “serendipitous” weights, the cost grows linearly with both dimension and number of lattice points, allowing practical computations in 1,000 dimensions, and no curse of dimensionality.

## [01697] QMC and sparse grids beyond uniform distributions on cubes

**Format :** Talk at Waseda University

**Author(s) :** Ilja Klebanov (Free University of Berlin) Tim Sullivan (University of Warwick)

**Abstract :** While Monte Carlo and MCMC methods are generally applicable and have a dimension-independent convergence rate, this rate is rather slow and unfeasible for many applications. Sparse grids and Quasi Monte Carlo methods provide better convergence rates under certain assumptions, but have only been constructed for uniform distributions on cubes and several other very specific distributions such as Gaussians. In this talk, I will show how these methods can be generalized to mixtures of such specific distributions, e.g. Gaussian mixtures, by means of a properly constructed transport map, which is a crucial step towards combining QMC and sparse grids methods with state of the art importance sampling algorithms, that are often based on such mixtures. I will avoid technical details and present lots of illustrations and videos instead.

## [02052] Can hyperinterpolation part with quadrature exactness?

**Format :** Online Talk on Zoom

**Author(s) :** Congpei An (Southwestern University of Finance and Economics)Hao-Ning Wu (The Hong Kong University)

**Abstract :** We discuss the approximation of continuous functions on the unit sphere by spherical polynomials of degree  $n$  via hyperinterpolation. Hyperinterpolation of degree  $n$  is a discrete approximation of the  $L^2$ -orthogonal projection of degree  $n$  with its Fourier coefficients evaluated by a positive-weight quadrature rule that exactly integrates all spherical polynomials of degree at most  $2n$ . This talk aims to bypass this quadrature exactness assumption by replacing it with the Marcinkiewicz-Zygmund property. Consequently, hyperinterpolation can be constructed by a positive-weight quadrature rule--not necessarily with quadrature exactness. This scheme is called unfettered hyperinterpolation. We provide a reasonable error estimate for unfettered hyperinterpolation. The error estimate generally consists of two terms: a term representing the error estimate of the original hyperinterpolation of full quadrature exactness and another introduced as compensation for the loss of exactness degrees. A guide to controlling the newly introduced term in practice is provided. In particular, if the quadrature points form a quasi-Monte Carlo design, then there is a refined error estimate. Numerical experiments verify the error estimates and the practical guide.

## [04553] Quasi-Monte Carlo-Based Algorithms for Deep Learning with Applications

**Format :** Online Talk on Zoom

**Author(s) :** Xiaoqun Wang (Tsinghua University)

**Abstract :** Deep learning methods are now used to solve (stochastic) partial differential equations in high dimensions, where the loss functions are defined as mathematical expectations. Traditional method to approximate the expectation is Monte Carlo (MC) method. We propose novel deep learning algorithms based on quasi-Monte Carlo (QMC) method, which is a deterministic version of MC method. We prove that the theoretical convergence order of QMC-based deep learning algorithms is asymptotically higher than that of MC-based algorithms. Numerical experiments demonstrate the substantial superiority of QMC-based algorithms in various applications.

00652 (3/3) : 5D @G304 [Chair: Takashi Goda]

## [04614] Lattice rules for integration on $\mathbf{R}^d$

**Format :** Talk at Waseda University

**Author(s) :** Dirk Nuyens (KU Leuven)

**Abstract :** For integration of periodic functions of mixed smoothness on the unit cube lattice rules are a very good choice. Their group theoretical structure allows for a convenient error analysis.

When integrating functions on  $\mathbb{R}^d$  there are multiple ways of still making use of lattice rules. We could truncate the integration region, and take into account the truncation error and the projection distance to the periodic subspace; or we could do a substitution and map the integrand to the unit cube. Depending on how we proceed it is possible to retain the smoothness and obtain higher order convergence with a lattice rule.

## [04320] SNPE-B Revisited: Rethinking of Data Efficiency and Variance Reduction

**Format :** Talk at Waseda University

**Author(s) :** Zhijian He (South China University of Technology)

**Abstract :** Sequential neural posterior estimation (SNPE) techniques have recently proposed for dealing with simulation-based models with intractable likelihoods. Unlike approximate Bayesian computation, SNPE techniques learn the posterior from sequential simulation using neural network-based conditional density estimators. This paper reclaims the efficiency of SNPE-B proposed by Lueckmann et al. (2017) through sophisticated sampling strategies. We firstly introduce a concentrated loss function based on an adaptive calibration kernel that reweights the simulated data appropriately to improve the data efficiency. We also provide a theoretical analysis of the variance of importance sampling-based estimators. We then propose several variance reduction techniques including quasi-Monte Carlo sampling to further accelerate the process of learning. Numerical experiments demonstrate that our method outperforms the original SNPE-B method together with other existing competitors on certain tasks.

## [04916] Variable importance measures in high dimensional data sets

**Format :** Talk at Waseda University

**Author(s) :** Art B Owen (Stanford University)

**Abstract :** This talk connects some ideas from QMC sampling to new problems in explainable AI. Variable importance measures in global sensitivity analysis are commonly derived from the ANOVA decomposition. The ANOVA is problematic with dependent variables. Then Shapley values and related quantities are used to measure importance, and those can be studied through the anchored decomposition, also common in quasi-Monte Carlo sampling.

Based on work with Ben Seiler, Christopher Hoyt, Masayoshi Mase and Naofumi Hama.

## [03703] Tuning QMC point sets using WAFOM-like value

**Format :** Talk at Waseda University

**Author(s) :** Makoto Matsumoto (Hiroshima University)

**Abstract :** There are many figures of merit for QMC point set  $P$ . The star discrepancy  $D^*(P)$  is a famous one. We restrict ourself to the case of 2-adic digital nets. Then,  $P$  can be considered as an  $F_2$ -vector space, where  $F_2$  is the two-element field. Let  $P'$  be the perpendicular space of  $P$ . Then,  $P'$  is considered as the space of linear relations satisfied by  $P$ . As a rough sketch,  $P$  is more uniform if any non-zero element  $A$  in  $P'$  is sufficiently complicated. One way to measure the complexity of  $A$  is Niederreiter-Rosenbloom-Tsfasman (NRT) weight; the smallest NRT weight among all possible non-zero weights gives the  $t$ -value. As other figures of merits, we may consider Dick weight  $\mu_{\alpha}(A)$  of  $A$  in  $P'$ . Summation of  $2^{-\mu_{\alpha}(A)}$  over nonzero  $A$  in  $P'$  gives figures of merit studied by Dick, and by considering the limit where  $\alpha$  goes to infinity, we obtain WAFOM. It is used by Harase that NRT weight is invariant by lower triangular transformation, but WAFOM differs, and so one can obtain better performance for smooth integrand when WAFOM is optimized while  $t$ -value is fixed. We study a justification of this method, and variation where Dick weight is replaced with NRT weight.

# [00654] Poset Combinatorics

**Session Time & Room :** 2D (Aug.22, 15:30-17:10) @G302

**Type :** Proposal of Minisymposium

**Abstract :**

To a finite poset  $P$  we associate two algebraic objects: the order polynomial  $\Omega(P, n)$ , which counts the number of order preserving labeling maps of posets from  $P$  to  $1 < 2 < \dots < n$ ; and the generating series  $\sum \Omega(P, n)x^n$ , called order series.

This algebraic setting leads to interactions with operad theory, metric spaces, cellular automata, and combinatorial species. In this mini-symposium, the experts will introduce those tools and expose their contributions as well as open questions. The talks will include theoretical results as well as applications to nonlinear signal-flow graphs.

**Organizer(s) :** Eric Rubiel Dolores-Cuenca

**Classification :** 05a15, 06a11, 18m80

**Minisymposium Program :**

00654 (1/1) : 2D @G302 [Chair: Eric Rubiel Dolores Cuenca]

## [02151] The operad of finite posets acts on zeta values

**Format :** Talk at Waseda University

**Author(s) :** Eric Dolores Cuenca (Yonsei University)

**Abstract :** Consider Riemann zeta function  $\zeta(k) = \sum_{n=1}^{\infty} \frac{1}{n^k}$ . We develop a theory in which the zeta values and the order polytopes share the same combinatorial information. More precisely, we show that the operad of finite posets acts on Stanley order polynomials, and the aforementioned operad acts on a set of numbers generated by zeta values. To demonstrate that the action of the operad on zeta values is not trivial, we explicitly compute a quaternary associative non commutative operation.

## [01777] What is $-Q$ for a poset $Q$ ?

**Format :** Talk at Waseda University

**Author(s) :** Masahiko Yoshinaga (Osaka University)

**Abstract :** In the context of combinatorial reciprocity, it is a natural question to ask what " $-Q$ " is for a poset  $Q$ . In a previous work, the definition " $-Q := Q \times R$  with lexicographic order" was proposed based on the notion of Euler characteristic of semialgebraic sets. In fact, by using this definition, Stanley's reciprocity for order polynomials was generalized to an equality for the Euler characteristics of certain spaces of increasing maps between posets. The purpose

part\_1

of this paper is to refine this result, that is, to show that these spaces are homeomorphic if the topology of  $Q$  is metrizable.

## [04172] A new expression for the order polynomial

**Format :** Online Talk on Zoom

**Author(s) :** Fengming Dong (Nanyang Technological University)

**Abstract :** In 1970s, Stanley introduced the order polynomial of a poset  $P$ . For a poset  $P$ , a mapping  $\sigma : P \rightarrow [m]$  is said to be order-preserving if  $u \preceq v$  implies that  $\sigma(u) \leq \sigma(v)$ . The order polynomial  $\Omega(P, x)$  is defined to be the function which counts the number of order-preserving mappings  $\sigma : P \rightarrow [m]$  whenever  $x = m$  is a positive integer. In this talk, I will introduce an expression for  $\Omega(P, x)$ , and an expression for the chromatic polynomial of a graph by applying this new result on order polynomial.

## [02099] Polychrony as chinampas

**Format :** Online Talk on Zoom

**Author(s) :** José Antonio Arciniega-Nevárez (Universidad de Guanajuato)

**Abstract :** In this talk, we will discuss the effect of stimulating some nodes at certain time (initial condition) in a signal flow path with auto-edges. The stimuli are applied at different times. The effect of these stimuli propagates through the vertices of the path, causing other nodes, which we will call secondary nodes, to cascade. We are interested in cascades in which the initial stimuli are less than or equal to the number of secondary vertices. This can be transferred to the study of a graph with weights, these weights being the times at which a signal travels from the output vertex to the arrival vertex. We are interested in knowing the time at which a node will be activated under a certain initial condition. The problem is nonlinear, so to deal with time, we propose to study a latiz, where, vertically, the time is described and horizontally, the vertices of the path are repeated. In this way, a vertex of the latiz will be connected to another one to which it was already connected in the path but at a different height, depending on the time.

If the time is always  $t=1$ , the problem becomes to study an automaton, where a cell at time  $t$  lives depending on the cells alive at time  $t-1$ , in particular we are interested in the rule 192 with the difference that the automaton is reactivated at different times (with the initial condition). The generated automata, that we call chinampas, have topological and combinatorial properties that allow us to solve the initial problem. Moreover, we can characterize automata in which the number of cells outside the initial condition are equal to or one more than those of the initial condition.

For the case in which we have more than one of these cells, we have translated the problem to one of triangular series with order conditions. These series can be obtained from partially ordered sets (posets). We have noted that the series obtained are known as generalizations of Stanley polynomials whose coefficients count the different ways of labeling a poset preserving the order.

The problem was inspired by the behavior of a neural network so this work is related to those who study such neural networks as polychrony groups, in fact, this is a particular case of polychrony.

## [00656] Multiscale Pattern Formation

**Session Time & Room :**

00656 (1/3) : 1D (Aug.21, 15:30-17:10) @G501

00656 (2/3) : 1E (Aug.21, 17:40-19:20) @G501

00656 (3/3) : 2C (Aug.22, 13:20-15:00) @G501

**Type :** Proposal of Minisymposium

**Abstract :** One way to understand the complex dynamics in dissipative systems is to decompose the object into subsystems with different spatiotemporal scales. The resulting subsystems could be unified by singular perturbation, fast-slow method, unfolding of singularities, bifurcation, and data-driven approaches. We collect 12 talks to present the state-of-the-art multi-scale pattern formation arising in biology, chemical reaction, fluid dynamics, and materials science in homogeneous and heterogeneous media. One of our goals is to find a promising direction in the newly emerging field of multiscale pattern formation problems.

**Organizer(s) :** Yasumasa Nishiura, Arjen Doelman

**Classification :** 35B36, 35B32, 37L10, 92E20, 92B99

**Minisymposium Program :**

00656 (1/3) : 1D @G501 [Chair: Arjen Doelman]

## [01951] Multiscale pattern formation in space and time

**Format :** Talk at Waseda University

**Author(s) :** Yasumasa Nishiura (Hokkaido University/Chubu University)

**Abstract :** One way to understand the complex dynamics in dissipative systems is to decompose the object into subsystems with different spatiotemporal scales. The resulting subsystems could be unified by singular perturbation, fast-slow method, unfolding of singularities, bifurcation, averaging, and data-driven approaches. I will try to present the state-of-the-art multi-scale pattern formation arising in biology, chemical reaction, fluid dynamics, and materials science in homogeneous and heterogeneous media.

## [01983] Localized spot dynamics: curvature and instability

**Format :** Talk at Waseda University

**Author(s) :** Justin Tzou (Macquarie University)

**Abstract :** For localized spots solutions of singularly perturbed reaction-diffusion systems, we discuss two aspects of slow drift dynamics: the oscillatory instabilities, and effects of domain curvature. The problem with curvature is analyzed within the context of a model of vegetation patterns on a curved terrain, which incorporates advection effects due to flow of water downhill. The stability analysis on flat domains centers on understanding how domain geometry selects dominant modes of oscillation.

## [01901] Spiky patterns in a three-component consumer chain model

**Format :** Talk at Waseda University

**Author(s) :** Shuangquan Xie (Hunan University)

**Abstract :** We study a cooperative consumer chain model with one producer and two consumers, which is a three-component extension of the Schankenberg model. We show that consumers can survive and have a profile of a spike for sufficiently high consumption. We then study the stability of spike solutions. When the consumption constant is further increased to a certain threshold, the system undergoes a Hopf bifurcation and the spiky pattern begins to oscillate.

## [01941] Emergence of locomotion by autonomous parameter tuning

**Format :** Talk at Waseda University

**Author(s) :** Keiichi Ueda (University of Toyama)Takumi Horita (University of Toyama)

**Abstract :** A peristaltic locomotion model with parameter tuning is presented. The parameter tuning system is described by the dynamical system with selection algorithm. The model autonomously generates stable elongation-contraction wave and finds appropriate anchor timing. We model the parameter tuning system as distributed system in order that the system achieves adaptability to various environmental changes.

00656 (2/3) : 1E @G501 [Chair: Edgar Knobloch]

## [01917] Symmetry-Breaking for a Compartmental-Reaction Diffusion System

**Format :** Talk at Waseda University

**Author(s) :** Michael Ward (University of British Columbia)

**Abstract :** We investigate pattern formation for a 2D PDE-ODE bulk-cell model, where two bulk diffusing species are coupled to nonlinear intracellular reactions that are confined within a disjoint collection of small circular compartments within the domain. The bulk species are coupled to the spatially segregated intracellular reactions through Robin conditions across the cell boundaries. For this compartmental-reaction diffusion system, symmetry-breaking bifurcations, regulated by a membrane binding rate ratio, occur even when the bulk species have equal diffusivities.

## [01765] Bayesian Model Selection of PDEs for Pattern Formation

**Format :** Talk at Waseda University

**Author(s) :** Natsuhiko Yoshinaga (Tohoku University)Satoru Tokuda (Kyushu University)

**Abstract :** Partial differential equations (PDEs) have been widely used to reproduce patterns in nature and to give insight into the mechanism underlying their formation. PDE models often rely on the pre-request knowledge of physical laws and developing a model to reproduce a desired pattern remains difficult. We propose a method to estimate the best PDE from one snapshot of an objective pattern under the stationary state. We apply our method to complex patterns, such as quasi-crystals.

**[02979] Spectral Stability of Far-from-Equilibrium Planar Periodic Patterns****Format :** Online Talk on Zoom**Author(s) :** Björn de Rijk (Karlsruhe Institute of Technology)

**Abstract :** We consider the existence and spectral stability of far-from-equilibrium planar periodic patterns in reaction-diffusion-advection systems. The planar periodic traveling waves are constructed by bifurcating from one-dimensional wave trains undergoing a transverse short-wave destabilization. The selected wavenumber matrix and velocity vector at bifurcation are fully determined by the wavenumber, velocity and critical Bloch modes of the underlying wave train. Our spectral analysis of the planar periodic pattern yields an expansion of the critical spectral surface touching the origin due to translational invariance in both spatial directions. In particular, such an expansion allows for an explicit verification of the spectral stability conditions implying nonlinear stability of the planar periodic pattern against spatially localized perturbations. This is joint work with Miguel Rodrigues (Université de Rennes 1, France).

**[01867] Fronts in the wake of a slow parameter ramp****Format :** Online Talk on Zoom**Author(s) :** Ryan Goh (Boston University) Tasso Kaper (Boston University) Arnd Scheel (University of Minnesota) Theodore Vo (Monash University)

**Abstract :** We discuss front solutions in the presence of a parameter ramp which slowly varies in space, rigidly propagates in time, and moderates the (in)stability of a spatially-homogeneous equilibrium, nucleating a traveling wave in its wake. For moving ramps, the front location is governed by a slow passage between convective and absolute instability; a projectivized fold. For stationary ramps, fronts are governed by slow-passage through a pitchfork and a connecting solution of the Painlevé-II equation.

00656 (3/3) : 2C @G501 [Chair: Michael Ward]

**[02507] Front propagation in a multi-variable morphogenetic model of branching****Format :** Talk at Waseda University**Author(s) :** Edgar Knobloch (University of California at Berkeley) Arik Yochelis (Ben-Gurion University of the Negev)

**Abstract :** We study the existence and stability of propagating fronts in the Meinhardt model of branching in 1D. We identify a sniper bifurcation of fronts that leads to episodic front propagation in the parameter region below propagation failure and show that this state is stable. We show that propagation failure is a consequence of a T-point in a spatial dynamics description and identify additional T-points responsible for a large multiplicity of different traveling front-peak states.

**[02105] CONTROL OF ENGULFMENT FOR BINARY POLYMER PARTICLES****Format :** Talk at Waseda University**Author(s) :** Takashi Teramoto (Asahikawa Medical University)

**Abstract :** Engulfment configurations with separated phases occur in the nanoparticles of a binary polymer mixture. Numerical investigations of the Cahn-Hilliard model with the boundary contact energy show the relationships between the free energies and two types of configurations within confined spheres in three-dimensions. These results are consistent with experimental observations. A Janus-type configuration forms a spherical-cap-shaped interface inside a particle. In the core-shell configuration, one of polymer phases completely engulfs another phase to form concentric interfaces with inner and outer phases. We consider the sharp interface limit of equilibrium configurations and derive the stability condition that each configuration becomes the only minimizer when the contact angle changes between the three phases.

**[03494] Instability of Planar Interfaces in Reaction-Diffusion-Advection Equations****Format :** Talk at Waseda University**Author(s) :** Paul Carter (University of California, Irvine)

**Abstract :** We consider planar interfaces between stable homogeneous rest states in singularly perturbed 2-component reaction diffusion advection equations, motivated by the appearance of fronts between bare soil and vegetation in dryland ecosystems, as well as multi-interface solutions, such as vegetation stripes. On sloped terrain, one can find stable traveling interfaces, while on flat ground, one finds that sideband instabilities along the interface can lead to labyrinthine Turing-like patterns. To explore this behavior, using geometric singular perturbation methods, we analyze instability criteria for planar interfaces in reaction diffusion advection systems, focussing on a specific Klausmeier-type model, and examine the effect of terrain slope on the stability of the interfaces.

## [04510] Patterns on patterns

**Format :** Online Talk on Zoom

**Author(s) :** Martina Chirilus-Bruckner (Leiden University)Jolien Kamphuis (Leiden University)

**Abstract :** The formation of patterns on top of spatially varying background states in the context of reaction-diffusion systems with spatially varying coefficients (such as the extended Klausmeier model) is motivated by the study of vegetation patterns on changing topographies. We present two regimes: (i) At onset when the background state loses stability and small amplitude modulations occur and (ii) in the long wavelength limit where the patterned state is composed of highly localized individual pulses.

## [00657] Tomographic inverse problems and deep learning techniques

**Session Time & Room :** 3E (Aug.23, 17:40-19:20) @F401

**Type :** Proposal of Minisymposium

**Abstract :** Tomographic inverse problems involve the recovery of physical quantity (shown as image) from indirect observations. These inverse problems are typically ill-posed and there have been numerous attempts to obtain the proper solution based on mathematical modeling. Deep learning has recently emerged as a powerful tool for solving the inverse problem, as it demonstrates the potential to handle uncertainty of the solution with large amounts of training data. In this mini-symposium, we will discuss mathematical and deep learning strategies for solving inverse problems related to imaging modalities such as computed tomography (CT), magnetic resonance imaging (MRI), and electrical impedance tomography (EIT).

**Organizer(s) :** Kiwan Jeon, Hyoung Suk Park, Jin Keun Seo

**Classification :** 49N45, 68T07, 92C55

**Minisymposium Program :**

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00657 (1/1) : 3E @F401 [Chair: Kiwan Jeon]

## [05264] Ill-posed Inverse problems in Low-dose Dental Cone-beam Computed Tomography

**Format :** Talk at Waseda University

**Author(s) :** Hyoung Suk Park (National Institute for Mathematical Sciences)Chang Min Hyun (Yonsei University)Jin Keun Seo (Yonsei University)

**Abstract :** Dental cone-beam computed tomography (CBCT) has been increasingly being used in various dental fields such as implant/prosthetics, oral and maxillofacial surgery, and orthodontic treatment. It aims to provide high-resolution images with the lowest possible radiation dose at a low cost for equipment. However, this cost-competitive goal makes the inverse problem of dental CBCT more nonlinear and ill-posed. In this presentation, we describe the mathematical structure of an ill-posed nonlinear inverse problem of low-dose dental CBCT and explain the advantages and limitations of the deep learning-based approach for CBCT image reconstruction compared to conventional regularization methods.

## [05265] Machine learning for automatic signal quality assessment in multi-channel electrical impedance-based hemodynamic monitoring

**Format :** Talk at Waseda University

**Author(s) :** Chang Min Hyun (Yonsei University)

**Abstract :** Owing to recent advances in thoracic electrical impedance tomography, a patient's hemodynamic function can be noninvasively and continuously estimated in real-time by surveilling a cardiac volume signal associated with stroke volume and cardiac output. In clinical applications, however, a cardiac volume signal is often of low quality, mainly because of the patient's deliberate movements or inevitable motions during clinical interventions. This talk deals with developing a signal quality indexing method that assesses the influence of motion artifacts on transient cardiac volume signals. We apply divergent machine-learning methods from discriminative-model to manifold learning. The use of machine-learning could be suitable for our real-time monitoring application that requires fast inference and automation as well as high accuracy. In the clinical environment, the proposed method can be utilized to provide immediate warnings so that clinicians can minimize confusion regarding patients' conditions, reduce clinical resource utilization, and improve the confidence level of the monitoring system. Numerous experiments using actual EIT data validate the capability of cardiac volume signals degraded by motion artifacts to be accurately and automatically assessed in real-time by machine learning.

## [05332] Application of AI-based Medical Diagnosis: focusing on tomography

**Format :** Talk at Waseda University

**Author(s) :** Soomin Jeon (Dong-A University)

**Abstract :** In this talk, we will see the various applications of artificial intelligence (AI) based medical diagnosis, focusing on tomography. From data set configuration for AI medical image research using tomography such as PET, X-ray, and X-ray CT, we look at the results of research on training algorithms. We also cover research related to the latest diagnostic technologies such as Alzheimer's disease.

## [05324] Data-driven reconstruction in X-ray CT with provable convergence guarantees

**Author(s) :** Jürgen Frikel (OTH Regensburg) Simon Göppel (University of Innsbruck) Markus Haltmeier (University of Innsbruck)

**Abstract :** Computed tomography (CT) is a widely used imaging technique in various fields including medicine, engineering, and materials science. CT image reconstruction is an ill-posed problem, which means that small errors in the measurements can lead to significant errors in the reconstruction. In order to stabilize the image reconstruction, the use of regularization techniques is crucial. Classical regularization methods (e.g., variational regularization) are known to provide convergent methods, but the resulting reconstructions may not be optimal. On the other hand, regularization strategies based on machine learning methods have been shown to produce better reconstructions, but often lack theoretical convergence guarantees. To address these challenges, we propose a convergent data-driven reconstruction method for x-ray tomography. Our framework consists of two steps, where in a classical regularization is used in the first step and a deep learning approach is used in the second step. Both steps are coupled by integrating data proximity into a network architecture. This integration allows us to leverage the strengths of both approaches while addressing their limitations. Our experimental results demonstrate the effectiveness of our approach in improving the accuracy of CT image reconstruction, while providing convergence guarantees.

## [00666] Simulations and Algorithms for Materials Sciences

**Session Time & Room :**

00666 (1/3) : 1C (Aug.21, 13:20-15:00) @D101

00666 (2/3) : 1D (Aug.21, 15:30-17:10) @D101

00666 (3/3) : 1E (Aug.21, 17:40-19:20) @D101

**Type :** Proposal of Minisymposium

**Abstract :** Simulation and computational methodologies are the third pillar alongside theory and experiment in materials science and engineering. Multiphysics and multiscale modeling and simulations incorporating proper numerical techniques and algorithms are key to understand the fundamental mechanisms in controlling the macroscopic material behaviors and make predictions. The development requires interdisciplinary collaborations and efforts, including applied physics, materials science, solid mechanics and applied mathematics. We propose a minisymposium in three sessions, with the aim of bringing together experts from diverse communities to share recent advances and research highlights in the understanding of this topic from their respective perspectives.

**Organizer(s) :** Yejun Gu, Zecheng Gan, Shidong Jiang

**Classification :** 74Q10, 35Q74, 65N30, 70G60, 82M31, Materials Science

**Minisymposium Program :**

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00666 (1/3) : 1C @D101 [Chair: Shidong Jiang]

## [02135] ESES, a Eulerian and Lagrangian molecular surface generator

**Format :** Talk at Waseda University

**Author(s) :** Weihua Geng (Southern Methodist University)

**Abstract :** The Poisson-Boltzmann (PB) model is numerically solved either on grid based meshes using finite difference/element methods or on body-fitted meshes using boundary element methods. In this talk, we investigate the distinguished features of the Eulerian Solvent Excluded Surface (ESES) software with which both Eulerian and Lagrangian surfaces are produced. We investigate the performance with these two types of surface discretization using the grid based MIBPB solver and body-fitted TABI-PB solvers.

## [02756] From nanocrystals to glasses: a strengthening mechanism analysis for amorphization.

**Format :** Talk at Waseda University

**Author(s) :** Chuqi CHEN (Hong Kong University of Science and Technology) Yang Xiang (Hong Kong University of Science and Technology)

**Abstract :** Recently, many studies investigated the correlation between the strength of the polycrystals, and the grain size and grain boundary width through both experimental and molecular dynamics simulation approaches. Results reveal that as grain boundary width increases, the crystalline structure of the grain boundary region transforms into an amorphous state. We propose mechanism analysis to elucidate the underlying mechanisms that govern the aforementioned relationships.

## [02794] Sum-of-Gaussians method with applications to molecular dynamics simulations

**Format :** Talk at Waseda University

**Author(s) :** Jiuyang Liang (Shanghai Jiao Tong University)

**Abstract :** Sum-of-Gaussians (SOG) method has attracted attention in many applications. In this talk, we will review some recently-developed SOG methods. Based on a sum-of-Gaussians decomposition of the Coulomb kernel, we develop an accurate, highly efficient, and scalable random batch sum-of-Gaussians (RBSOG) method for molecular dynamics simulations of systems with long-range interactions. Numerical results, including SPC/E bulk water and phase-separated electrolytes, are presented to show the attractive performance of the algorithm, including the superscalability in parallel computing.

## [03201] Random-batch Ewald method for molecular dynamics

**Format :** Talk at Waseda University

**Author(s) :** Zhenli Xu (Shanghai Jiao Tong University)

**Abstract :** We present a random-batch Ewald method for molecular dynamics of particle systems with long-range interactions. It takes advantage of the random minibatch strategy for particles, leading to an order N algorithm. It is based on the Ewald splitting of the Coulomb kernel and the random importance sampling is employed in the Fourier part such that the force variance can be reduced. Numerical results are presented to show the attractive performance of the algorithm.

00666 (2/3) : 1D @D101 [Chair: Zecheng Gan]

## [04335] Molecular Dynamics Simulation of Concentrated Entangled Polymers in Athermal Solvents

**Format :** Talk at Waseda University

**Author(s) :** Jiayi wang (HKUST)

**Abstract :** We have developed a coarse-grained model to simulate the geometric and dynamical properties of entangled polymer chains dissolved in athermal solvents. Our model successfully verifies the concentration scaling relationships of the geometric characteristics. In terms of the dynamical aspect, we have discovered that the swelling of the entangled polymer chains in athermal solvents leads to enhanced local chain stiffness or effective system elastic modulus.

## [04386] Multiscale modeling and Simulations of Interfacial Defects in based on PN model

**Author(s) :** Shuyang Dai (Wuhan University)

**Abstract :** A multiscale continuum model is developed to describe the defect structures in crystalline material such as FCC metals. The interface structure for twist, tilt and misfit grain boundaries are described by the dislocation network. The model incorporates both the anisotropy elasticity of each grain in crystalline materials and the molecular dynamics calculation informed interaction between two bulks, i.e., the nonlinear generalized stacking-fault energy. The equilibrium structures are obtained from the numerical simulations of the force balance differential equations. We apply this approach to determine the structure and energetics of twist, tilt and general grain boundaries. We also investigated the dislocation structure in heterogeneous crystalline material. Our model agrees well with the atomistic results. An analytical description is developed based on the obtained structural features.

## [04817] Solving integral equations on non-smooth boundaries

**Format :** Talk at Waseda University

**Author(s) :** Shidong Jiang (Center for Computational Mathematics, Flatiron Institute, Simons Foundation)Johan Helsing (Lund University)

**Abstract :** A numerical scheme is presented for the solution of Fredholm second-kind boundary integral equations on non-smooth boundaries. The scheme, which builds on recursively compressed inverse preconditioning (RCIP), is universal as it is independent of the nature of the singularities. The performance of the scheme is illustrated via several numerical examples.

## [05284] A fast algorithm for Dirichlet partition problems

**Format :** Talk at Waseda University

**Author(s) :** Dong Wang (The Chinese University of Hong Kong, Shenzhen)

**Abstract :** A Dirichlet k-partition of a domain is a collection of k pairwise disjoint open subsets such that the sum of their first Laplace–Dirichlet eigenvalues is minimal. In this talk, we propose a new relaxation of the problem by introducing auxiliary indicator functions of domains and develop a simple and efficient diffusion generated method to compute Dirichlet k-partitions for arbitrary domains. The method only alternates three steps: 1. convolution, 2. thresholding, and 3. projection. The method is simple, easy to implement, insensitive to initial guesses and can be effectively applied to arbitrary domains without any special discretization. At each iteration, the computational complexity is linear in the discretization of the computational domain. Moreover, we theoretically prove the energy decaying property of the method. Experiments are performed to show the accuracy of approximation, efficiency and unconditional stability of the algorithm. We apply the proposed algorithms on both 2- and 3-dimensional flat tori, triangle, square, pentagon, hexagon, disk, three-fold star, five-fold star, cube, ball, and tetrahedron domains to compute Dirichlet k-partitions for different k to show the effectiveness of the proposed method. Compared to previous work with reported computational time, the proposed method achieves hundreds of times acceleration.

00666 (3/3) : 1E @D101

## [00669] Mathematical Solutions of Industrial Applications

**Session Time & Room :** 3C (Aug.23, 13:20-15:00) @G404

**Type :** Proposal of Industrial Minisymposium

**Abstract :** Mathematics plays an important role in modern industry, for instance, as a tool for research & development and as algorithmic parts of products. This session presents success stories of industrial mathematics as a solution to various business challenges. Several domains of industry are considered: automotive, optics, manufacturing, medical imaging and agriculture. The following specific topics are included: 1. Data-driven development in industry, 2. Industrial applications of machine learning, 3. Inverse problems in medical X-ray imaging, 4. Machine learning in industry. Each talk will discuss the motivation, approaches and implementations based on mathematics.

**Organizer(s) :** Takanori Ide, Samuli Siltanen,

**Classification :** 34M50, 68U10, 65M20, Machine Learning

**Minisymposium Program :**

00669 (1/1) : 3C @G404 [Chair: Takanori Ide]

## [02716] Prediction of Leaf Area Index of Tomato Plants by Image Processing and Deep Learning

**Format :** Talk at Waseda University

**Author(s) :** Mario Tsukassa Sato (University of Tsukuba)Aiga Goto (University of Tsukuba)Nanami Isoda (University of Tsukuba)Ayu Kaise (University of Tsukuba)Claus Aranha (University of Tsukuba)Akira Imakura (University of Tsukuba)Tetsuya Sakurai (University of Tsukuba)Naomichi Fujiuchi (Ehime University)Naoya Fukuda (University of Tsukuba)

**Abstract :** In this work, we study how to improve image recognition in greenhouse tomato plants using Machine Learning. We propose a method for non-destructively estimating the Leaf Area Index (LAI), as well as a method to improve the segmentation of different parts of the plant. Moreover, we discuss our investigation of three ways to estimate the relevant parts of the segmented image. Additionally, we investigated new methods to improve the task of semantic segmentation of the whole plant.

## [02893] Frequency based graph estimation for multivariate time-series

**Format :** Talk at Waseda University

**Author(s) :** Yuuya Takayama (Nikon Corporation)

**Abstract :** We propose a method to estimate an underlying graph structure from multivariate time-series data. This method is derived from the Dynamic Mode Decomposition (DMD) method so as to recover an exact graph from a solution of the graph wave equation. In our talk, we introduce its applications and discuss uncertainty of an estimated graph based on the mathematical equation.

## [02900] Passive Gamma Emission Tomography for Spent Nuclear Fuel

**Format :** Talk at Waseda University

**Author(s) :** Riina Virta (Radiation and Nuclear Safety Authority (STUK), and Helsinki Institute of Physics, University of Helsinki)Tatiana Alessandra Bubba (University of Bath)Mikael Moring (Radiation and Nuclear Safety Authority (STUK))Samuli Siltanen (Department of Mathematics and Statistics of the University of Helsinki)Tapani Honkamaa (Radiation and Nuclear Safety Authority (STUK))Peter Dendooven (Helsinki Institute of Physics, University of Helsinki)

**Abstract :** Spent nuclear fuel needs to be verified prior to geological disposal in a deep underground repository. In Passive Gamma Emission Tomography (PGET), the gamma radiation emitted by the fuel is recorded with highly collimated semiconductor detectors and 2D slice images of activity and attenuation are simultaneously reconstructed to account for the high self-attenuation of the material. General information about the object geometry is used as a prior to regularize the ill-posed inverse problem.

## [02901] Boundary estimation of the X-ray tomographic reconstruction using persistent homology

**Format :** Talk at Waseda University

**Author(s) :** Elli Karvonen (University of Helsinki)

**Abstract :** In some applications, one can only use limited-angle X-ray tomography, which results in a much more difficult reconstruction problem than a full-angle case. Despite an algorithm, all parts of the smooth boundaries of the target object cannot be detected stably. In this talk the new boundary estimation method, which utilizes complex wavelets and persistent homology, is presented. The latest results are shown and discussed.

# [00670] Financial Risk Management and Related Topics

**Session Time & Room :**

00670 (1/2) : 1C (Aug.21, 13:20-15:00) @D502

00670 (2/2) : 1D (Aug.21, 15:30-17:10) @D502

**Type :** Proposal of Minisymposium

**Abstract :** The development of mathematical models used in financial risk management over the past few decades has been remarkable, and it is certainly an area of applied mathematics where many important research topics remain to be explored. This mini-symposium will focus on discussing recent topics related to mathematical methods for quantitative financial risk management. Specifically, topics such as credit risk modeling, applications of stochastic analysis to risk management, risk measures, multivariate statistical modelings, and so on will be presented.

**Organizer(s) :** Hidetoshi Nakagawa, Suguru Yamanaka

**Classification :** 91-10

**Minisymposium Program :**

00670 (1/2) : 1C @D502 [Chair: Hidetoshi Nakagawa]

## [03276] Discrepancy between Regulations and Practice in Initial Margin Calculation

**Format :** Talk at Waseda University

**Author(s) :** Ryosuke Kitani (Hitotsubashi University)Hidetoshi Nakagawa (Hitotsubashi University)

**Abstract :** Counterparty risk remains at issue in OTC derivative transactions. Since it is difficult to calculate the initial margin according to the regulations, it has been calculated in practice using a simplified method "ISDA SIMM". In this study, we derive an approximate formula for some indicators of counterparty risk for a stochastic volatility model and

illustrate some numerical analyses to examine the effect of discrepancy between regulations and practice in margin calculation.

## [02781] Last Passage Time and its Applications in Risk Management

**Format :** Talk at Waseda University

**Author(s) :** Masahiko Egami (Kyoto University)Rusudan Kevkhishvili (Kyoto University)

**Abstract :** We decompose the Laplace transform of a regular transient diffusion's last passage time into a simple formula based on Green functions. This result allows us to bypass often hard calculations related to diffusions with switching parameters by reducing the problem to two processes without switching. The last passage time is not a stopping time because it looks into the future path of the process. We demonstrate its application in credit risk and loss-given-default distribution modeling.

## [04631] Construction and sample path properties of Brownian house-moving

**Format :** Talk at Waseda University

**Author(s) :** Kensuke Ishitani (Tokyo Metropolitan University)

**Abstract :** We are currently investigating higher-order chain rules for computing higher-order Greeks of barrier options, and we expect a stochastic process called "Brownian house-moving" to play an important role in their computation. Brownian house-moving is a Brownian bridge conditioned to stays between two curves. The purpose of this talk is to construct Brownian house-moving. Also studied are the sample path properties of Brownian house-moving.

## [02599] Stability of High Order Moments: a Risk Management Approach

**Format :** Talk at Waseda University

**Author(s) :** Olivier Arnaud Le Courtois (emlyon business school)Silvia Faroni (emlyon business school)

**Abstract :** Little research has been produced on the statistical reliability of high order moments. This work studies the stability of higher order moments in equity markets. We extend our study to conditional annual higher order moment using different quantiles. Our aim is to identify which moment is more stable over time, which leads to a more reliable assessment of the future market risk and thus to more robust investment and risk management practices.

00670 (2/2) : 1D @D502 [Chair: Suguru Yamanaka]

## [03952] Gross-revenue-based structural credit risk model

**Format :** Talk at Waseda University

**Author(s) :** Suguru Yamanaka (Aoyama Gakuin University)Hidetoshi Nakagawa (Hitotsubashi University)

**Abstract :** For calculation of firms' default probability, structural models are often used to formulate the stochastic variation of stock variables such as total assets and firm value. In contrast, we propose a new type of structural model based on gross revenue, a flow variable that reflects the income and expenditure of firms. We test the validity of the default probabilities calculated from our proposed model using data on Japanese firms.

## [03406] Insider vs. Outsider: Information and Enlargement of Filtrations

**Format :** Talk at Waseda University

**Author(s) :** Kiichi Kitajima (Mitsubishi UFJ Trust Investment Technology Institute Co., Ltd. & Graduate School of Economics, Hitotsubashi University)

**Abstract :** In this presentation, we introduce a stock price process where a large insider can control the price movement through trading. Under the condition that additional insider information is binary, the study establishes that the information drift is a martingale and that the model has a unique equivalent martingale measure when the insider optimizes their trading. We also characterize the stock's expected return by the insider and an outsider with limited information.

## [02711] Sparse factor model of high dimension

**Format :** Talk at Waseda University

**Author(s) :** Benjamin POIGNARD (Osaka University)Yoshikazu TERADA (Osaka University)

**Abstract :** We consider the estimation of factor model-based covariance matrix when the factor loading matrix is sparse. We develop a penalized estimating function framework to account for the identifiability of the factor loading matrix while fostering sparsity. We prove the oracle property of the penalized estimator for factor model, that is the penalization can recover the true sparse support and the estimator is asymptotically normal. These theoretical results are supported by simulations and real data experiments.

## [03676] On a measure of tail asymmetry for the bivariate skew-normal copula

**Format :** Talk at Waseda University

**Author(s) :** Toshinao Yoshioka (Tokyo Metropolitan University) Takaaki Koike (Hitotsubashi University) Shogo Kato (Institute of Statistical Mathematics)

**Abstract :** Asymmetry in the upper and lower tails is an important feature in modeling financial risk factors. We analyze asymptotic behavior of a measure of tail asymmetry at extremely large and small thresholds of the bivariate skew-normal copula. We numerically show, when the correlation or skewness parameters are around at the boundary values, some proposed asymptotic approximations are not suitable to compute the measure of tail asymmetry.

## [00672] Efficient inference for large and high-frequency data

**Session Time & Room :**

00672 (1/3) : 5B (Aug.25, 10:40-12:20) @E502

00672 (2/3) : 5C (Aug.25, 13:20-15:00) @E502

00672 (3/3) : 5D (Aug.25, 15:30-17:10) @E502

**Type :** Proposal of Minisymposium

**Abstract :** In this minisymposium, the notion of asymptotically efficient estimation and asymptotically efficient statistical decision is discussed for various models appearing in finance and econometrics.

For some applications, the data are acquired at high-frequency and in-fill observation scheme is considered. Here, asymptotical properties of the estimators for the parameters of the rough volatility models in quantitative finance and for the solutions of stochastic differential equations with jumps or with singular coefficients will be presented.

In other applications, the large sample observation scheme is used. Asymptotical efficient statistical decisions and estimations are introduced for time series in econometrics (FARIMA, Threshold AR).

**Organizer(s) :** Alexandre Brouste, Mathieu Rosenbaum

**Classification :** 62Fxx, 62Mxx, 62Cxx

**Minisymposium Program :**

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00672 (1/3) : 5B @E502 [Chair: Alexandre Brouste]

## [05600] Fast and asymptotically efficient inference for large and high-frequency data

**Format :** Talk at Waseda University

**Author(s) :** Alexandre Brouste (Le Mans Université)

**Abstract :** In this minisymposium, the notion of asymptotically statistical decision is discussed for various models appearing in finance and econometrics. In some applications, the large sample observation scheme is used. Asymptotical efficient statistical decisions and estimations are introduced for time series in econometrics (FARIMA, Threshold AR). For other applications, the data are acquired at high-frequency and in-fill observation scheme is considered. Asymptotical properties for the estimators of the parameters in the solutions of stochastic differential equations with jumps or with singular coefficients or in the rough volatility models in quantitative finance will be presented.

## [05624] On Adaptive Kalman Filtration

**Format :** Talk at Waseda University

**Author(s) :** Yury Kutoyants (Le Mans University)

**Abstract :** We consider a linear partially observed system. The coefficients of this system depend on some unknown parameter. We study the problems of the construction of adaptive Kalman-Bucy filtration equations in the asymptotic of large samples. The properties of the MLE and BE are described. The adaptive filter is constructed in two steps. First we propose a method of moments preliminary estimator. Then this estimator is used for construction of One-step MLE-process. Finally we construct an adaptive recurrent filter.

## [05359] Fast calibration of weak FARIMA models

**Format :** Talk at Waseda University

**Author(s) :** Youssef Esstafa (Le Mans Université )

**Abstract :** In this work, we investigate the asymptotic properties of Le Cam's one-step estimator for weak FARIMA models. For these models, noises are uncorrelated but neither necessarily independent nor martingale differences errors. We show under some regularity assumptions that the one-step estimator is strongly consistent and asymptotically normal with the same asymptotic variance as the least squares estimator. We show through simulations that the proposed estimator reduces computational time compared with the least squares estimator.

## [05613] Fast Inference for Stationary Time Series

**Format :** Talk at Waseda University

**Author(s) :** Samir BEN HARIZ (Le Mans Université)Marius Soltane (Université de Compiègne)Alexandre Brouste (Le Mans Université)Youssef Esstafa (Le Mans Université)

**Abstract :** Stationary processes are widely used to model temporal dependence in various random phenomena including Economy, Finance, Hydrology,... In the Gaussian case, statistical inference for such processes, which is well-known, often relies on the maximum likelihood estimation or its approximation using the Whittle method. The asymptotic variance is then optimal in both cases. However, these methods are generally computationally expensive or even extremely difficult to apply to large samples.

We propose an alternative which is computationally fast while keeping the same asymptotic properties both in terms of speed and asymptotic variance. The procedure consists of applying a so-called one-step method to an initial estimator that is easy to implement and satisfies a certain condition on its convergence rate.

The process begins by initializing the parameter estimate by a simple and eventually poor estimator. Once the initial estimates are determined, the iteration step begins. Using the score vector and the Fisher Information Matrix, the parameter estimates are updated. The updated estimates are obtained by taking a step proportional to the inverse of the Fisher Information Matrix multiplied by the score vector. The one-step estimation method is called so because it updates the parameter estimates only once per iteration. This makes it computationally efficient and relatively simple to implement compared to other more complex estimation methods.

We will start with the simplest case where the process is Gaussian and then generalize this procedure to non-Gaussian processes. We also illustrate the numerical performance of this method through simulations and compare it to classical methods.

00672 (2/3) : 5C @E502 [Chair: Laurent Denis]

## [03747] Local asymptotic property for the Euler approximation of SDE driven by a stable Lévy process

**Format :** Talk at Waseda University

**Author(s) :** Emmanuelle Clément (University Gustave Eiffel)Alexandre Brouste (Le Mans University)Thi Bao Trâm Ngô (Le Mans University)Laurent DENIS (Le Mans University )

**Abstract :** We study the stochastic differential equations driven by a symmetric stable Lévy process, in which the joint parametric estimation of the drift coefficient, the scale coefficient and the jump activity of the process based on high frequency observations on a fixed time interval is considered. For these experiments, due to the non-explicit form of the likelihood function, our methodology will be to identify a simpler experiment, where the likelihood function has a traceable form, which is asymptotically equivalent in the Le Cam distance at the process observed at high frequency. To cover all values of jumping activity, the most appropriate experiment is to consider a numerical scheme that combines Euler's approximation of the scale coefficient with the solution of the ordinary equation given by the coefficient of derivative. We therefore prove the LAMN property for this corresponding Euler scheme with the ordinary differential equation. Thanks to the obtained LAMN property, we show that the one-step estimator is efficient. With an easy-to-compute initial estimator with good asymptotic behavior, it can exhibit a performance quite similar to that of the maximum likelihood estimator and reduce a lot of computation time. We illustrate our results by numerical simulations with the one-step procedure.

## [03713] Asymptotics for Student-Lévy regression

**Format :** Talk at Waseda University

**Author(s) :** Hiroki Masuda (University of Tokyo)

**Abstract :** We consider the quasi-likelihood analysis for a linear regression model driven by a Student Lévy process with constant scale and arbitrary degrees of freedom. We consider joint estimation of trend, scale, and degrees of freedom when the model is observed at a high frequency over an extending period. The bottleneck in this problem is that the Student distribution is not closed under convolution, making it difficult to estimate all the parameters fully based on the high-frequency time scale. To efficiently deal with that intricate nature, we propose a two-step quasi-likelihood analysis:

first, we make use of the Cauchy quasi-likelihood for estimating the regression-coefficient vector and the scale parameter; then, we construct the sequence of the unit-period cumulative residuals to estimate the remaining degrees of freedom. We will present the hopefully asymptotically efficient theoretical behavior of the proposed estimator, which quantitatively clarifies the need for data thinning.

## [01903] High-frequency estimation of pure jump alpha-CIR process

**Format :** Talk at Waseda University

**Author(s) :** Elise Bayraktar (Université Gustave Eiffel)

**Abstract :** We consider a pure-jump stable Cox-Ingersoll-Ross ( $\alpha$ -stable CIR) process defined by

$X_t = x_0 + \int_0^t (a - bX_s) ds + \int_0^s \delta X_{s-}^{1/\alpha} dL_s^\alpha$  where  $(L_t^\alpha)_{t \geq 0}$  is a compensated  $\alpha$ -stable Lévy process with non-negative jumps and  $\alpha \in (1, 2)$ .

We study the joint estimation of drift, scaling and jump activity parameters  $(a, b, \delta, \alpha)$  from high-frequency observations of the process on a fixed time period. We prove the existence of a consistent and asymptotic mixed normal estimator based on an approximation of the likelihood function.

## [02309] Local asymptotic properties for the growth rate of a jump-type CIR process

**Format :** Online Talk on Zoom

**Author(s) :** Mohamed Ben Alaya (University of Rouen)Ahmed Kebaier (University of Evry)Gyula Pap (University of Szeged)Ngoc Khue Tran (Hanoi University of Science and Technology)

**Abstract :** In this paper, we consider a one-dimensional jump-type Cox-Ingersoll-Ross process driven by a Brownian motion

and a subordinator, whose growth rate is an unknown parameter. The Lévy measure of the subordinator is finite or infinite. Considering the process observed continuously or discretely at high frequency, we derive the local asymptotic properties for the growth rate in both ergodic and non-ergodic cases.

Three cases are distinguished: subcritical, critical and supercritical. Local asymptotic normality (LAN) is proved in the subcritical case, local asymptotic quadraticity (LAQ) is derived in the critical case, and local asymptotic mixed normality (LAMN) is shown in the supercritical case. To do so, techniques of Malliavin calculus and a subtle analysis on the jump structure of the subordinator involving the amplitude of jumps and number of jumps are essentially used.

00672 (3/3) : 5D @E502 [Chair: Mathieu Rosenbaum]

## [01940] Statistical inference for rough volatility: minimax theory

**Format :** Talk at Waseda University

**Author(s) :** Grégoire Szymanski (Ecole Polytechnique, CMAP)Carsten Chong (Columbia University, 1Department of Statistics)Marc Hoffmann (Université Paris Dauphine-PSL, Ceremade)Yanghui Liu (Baruch College CUNY, 3Department of Mathematics)Mathieu Rosenbaum (Ecole Polytechnique, CMAP)

**Abstract :** Rough volatility models have gained considerable interest in the quantitative finance community in recent years. In this paradigm, the volatility of the asset price is driven by a fractional Brownian motion with a small value for the Hurst parameter  $H$ . In this work, we provide a rigorous statistical analysis of these models. To do so, we establish minimax lower bounds for parameter estimation and design procedures based on wavelets attaining them. We notably obtain an optimal speed of convergence of  $n^{-1/(4H+2)}$  for estimating  $H$  based on  $n$  sampled data, extending results known only for the easier case  $H > 1/2$  so far. We therefore establish that the parameters of rough volatility models can be inferred with optimal accuracy in all regimes.

## [01388] Statistical inference for rough volatility: Central limit theorems

**Format :** Online Talk on Zoom

**Author(s) :** Carsten H. Chong (HKUST)Marc Hoffmann (Université Paris Dauphine-PSL)Yanghui Liu (Baruch College CUNY)Mathieu Rosenbaum (Ecole Polytechnique)Grégoire Szymanski (Ecole Polytechnique)

**Abstract :** In recent years, there has been substantive empirical evidence that stochastic volatility is rough. In other words, the local behavior of stochastic volatility is much more irregular than semimartingales and resembles that of a fractional Brownian motion with Hurst parameter  $H < 0.5$ . In this paper, we derive a consistent and asymptotically mixed normal estimator of  $H$  based on high-frequency price observations. In contrast to previous works, we work in a semiparametric setting and do not assume any a priori relationship between volatility estimators and true volatility. Furthermore, our estimator attains a rate of convergence that is known to be optimal in a minimax sense in parametric rough volatility models.

## [02004] A GMM approach to estimate the roughness of stochastic volatility

**Format :** Talk at Waseda University

**Author(s) :** Anine Bolko (Aarhus University) Kim Christensen (Aarhus University) Mikko Pakkanen (University of Waterloo) Bezirgen Veliyev (Aarhus University)

**Abstract :** I will present an approach to estimate log normal stochastic volatility models, including rough volatility models, using the generalised method of moments, GMM. In this GMM approach, estimation is done directly using realised measures, e.g., realised variance, avoiding the biases that arise from using a proxy of spot volatility. I will also present asymptotic theory for the GMM estimator, lending itself to inference, and apply the methodology to Oxford-Man realised volatility data.

## [01999] Asymptotically Efficient Estimation for Fractional Brownian Motion with Additive Noise

**Format :** Talk at Waseda University

**Author(s) :** Tetsuya Takabatake (Hiroshima University) Grégoire Szymanski (Ecole Polytechnique, CMAP)

**Abstract :** We will talk about an asymptotically efficient estimation of the Hurst index and the volatility parameter for a fractional Brownian motion with additive noise based on discrete observations. We will propose an asymptotically efficient estimator combining the ideas of the one-step method and a quadratic variation-type estimator using pre-averaged data.

# [00673] Recent advances in discontinuous Galerkin methods and the related applications

**Session Time & Room :**

00673 (1/2) : 2C (Aug.22, 13:20-15:00) @E703

00673 (2/2) : 2D (Aug.22, 15:30-17:10) @E703

**Type :** Proposal of Minisymposium

**Abstract :** Discontinuous Galerkin methods are widely employed in computational science and engineering fields, as they offer accurate and efficient simulations. In particular, discontinuous Galerkin methods offer appealing features including high-order approximation, hp adaptivity, and local mass conservations, which are particularly important for practical applications. The development, analysis, and applications of discontinuous Galerkin methods have stimulated significant research. The aim of this mini-symposium is to gather experts as well as junior researchers in the field to introduce recent achievements on discontinuous Galerkin methods and the related applications, as well as promote exchanges.

**Organizer(s) :** Eric Chung, Lina Zhao

**Classification :** 65M60, 65M15, 65M12

**Minisymposium Program :**

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00673 (1/2) : 2C @E703 [Chair: Eric Chung]

## [03246] Bound preserving DG methods for multi-species flow with chemical reactions

**Format :** Talk at Waseda University

**Author(s) :** Jie Du (Tsinghua University)

**Abstract :** For multispecies chemical reactive flows, the solutions have some physical bounds. The mass fraction does not satisfy a maximum principle and hence it is not easy to preserve the upper bound. Also, most of the bound-preserving techniques available are based on Euler forward method. For problems with stiff source, the time step will be significantly limited. In this work, we will construct third order conservative bound-preserving DG methods to overcome all these difficulties.

## [03960] Staggered discontinuous Galerkin methods for the Stokes problem on rectangular grids

**Format :** Talk at Waseda University

**Author(s) :** Hyea Hyun Kim (Kyung Hee University)Thien Binh Nguyen (Vietnamese-German University)Gung-Min Gie (University of Louisville)Chang-Yeol Jung (UNIST)

**Abstract :** A staggered DG (Discontinuous Galerkin) method, that was originally developed on triangular meshes, is extended to rectangular grids for the second order elliptic problems in the first, second, and fourth authors' previous work. On the rectangular grids, the higher order polynomials in higher dimensions can be easily formed without the need for meshing the physical domain. In this talk, we present the extension of our previous staggered DG method to the Stokes system and provide the optimal error estimate for the given polynomial order. Compared to the triangle based DG methods, we also obtain a better inf-sup stability result for the rectangular based DG methods. Numerical results are presented to confirm our optimal error estimate results.

## [02857] A mass conservative scheme for the coupled flow and transport

**Format :** Talk at Waseda University

**Author(s) :** Lina Zhao (City University of Hong Kong)Shuyu Sun (KAUST)

**Abstract :** In this talk, I will present a mass conservative scheme for the coupled Brinkman flow and transport, where the flow equations are discretized using staggered DG method and mixed FEM. As such, the interface conditions are naturally incorporated into the formulation. Then the transport equation is discretized using unwinding staggered DG methods. The optimal convergence error estimates for all the variables are carried out. Several numerical experiments are carried out to demonstrate the performance.

## [03078] hp-Multigrid preconditioner for a divergence-conforming HDG scheme for the incompressible flow problems

**Format :** Online Talk on Zoom

**Author(s) :** Guosheng Fu (University of Notre Dame)Wenzheng Kuang (University of Notre Dame)

**Abstract :** In this study, we present an hp-multigrid preconditioner for a divergence-conforming HDG scheme for the generalized Stokes and the Navier-Stokes equations using an augmented Lagrangian formulation. Our method relies on conforming simplicial meshes in two- and three-dimensions. The hp-multigrid algorithm is a multiplicative auxiliary space preconditioner that employs the lowest-order space as the auxiliary space, and we developed a geometric multigrid method as the auxiliary space solver. For the generalized Stokes problem, the crucial ingredient of the geometric multigrid method is the equivalence between the condensed lowest-order divergence-conforming HDG scheme and a Crouzeix-Raviart discretization with a pressure-robust treatment as introduced in Linke and Merdon (Comput. Methods Appl. Mech. Engrg., 311 (2016)), which allows for the direct application of geometric multigrid theory on the Crouzeix-Raviart discretization. The numerical experiments demonstrate the robustness of the proposed *hp*-multigrid preconditioner with respect to mesh size and augmented Lagrangian parameter, with iteration counts insensitivity to polynomial order increase. Inspired by the works by Benzi & Olshanskii (SIAM J. Sci. Comput., 28(6) (2006)) and Farrell et al. (SIAM J. Sci. Comput., 41(5) (2019)), we further test the proposed preconditioner on the divergence-conforming HDG scheme for the Navier-Stokes equations. Numerical experiments show a mild increase in the iteration counts of the preconditioned GMRes solver with the rise in Reynolds number up to  $10^3$ .

00673 (2/2) : 2D @E703 [Chair: Lina Zhao]

## [04124] Numerical Modelling of the Brain Poromechanics by High-Order Discontinuous Galerkin Methods

**Format :** Online Talk on Zoom

**Author(s) :** Paola Francesca Antonietti (Politecnico di Milano)Mattia Corti (Politecnico di Milano)Luca Dede' (Politecnico di Milano)Alfio Quarteroni (Politecnico di Milano)

**Abstract :** In this talk we introduce and analyze a discontinuous Galerkin method for the numerical modelling of the equations of Multiple-Network Poroelastic Theory (MPET) in the dynamic formulation. The MPET model can comprehensively describe functional changes in the brain considering multiple scales of fluids. Concerning the spatial discretization, we employ a high-order discontinuous Galerkin method on polygonal and polyhedral grids and we derive stability and a priori error estimates. The temporal discretization is based on a coupling between a Newmark  $\beta$ -method for the momentum equation and a  $\theta$ -method for the pressure equations. We present verification numerical results and perform a convergence analysis using an agglomerated mesh of a geometry of a brain slice. We also present a simulation in a three-dimensional patient-specific brain reconstructed from magnetic resonance images. The model presented in this paper can be regarded as a preliminary attempt to model perfusion in the brain.

## [03151] Cell-average based Neural Network method for time dependent PDEs

**Format :** Talk at Waseda University

**Author(s) :** Changxin Qiu (Ningbo University)Jue Yan (Iowa State University)

**Abstract :** Motivated by finite volume scheme, a cell-average based neural network method is proposed. The method is based on the integral or weak formulation of partial differential equations. Offline supervised training is carried out to obtain the optimal network parameter set, which uniquely identifies one finite volume like neural network method. Once well trained, the network method is implemented as a finite volume scheme and can adapt large time step size for solution evolution.

## [04606] A non-overlapping Schwarz algorithm for the HDG method

**Format :** Talk at Waseda University

**Author(s) :** Issei Oikawa (University of Tsukuba)

**Abstract :** This talk is concerned with a non-overlapping Schwarz algorithm for the hybridizable discontinuous Galerkin (HDG) method for the steady-state diffusion problem. We present several iterative algorithms based on the non-overlapping Schwarz domain decomposition method and their numerical results.

## [03898] Adaptive methods for fully nonlinear PDE

**Format :** Online Talk on Zoom

**Author(s) :** Iain Smears (University College London)

**Abstract :** Hamilton--Jacobi--Bellman and Isaacs equations are important classes of fully nonlinear PDE with applications from stochastic optimal control and two player stochastic differential games. In this talk, we present our recent proof of the convergence of a broad family of adaptive nonconforming DG and  $C^0$ -interior penalty methods for the class of these equations that satisfy the Cordes condition in two or three space dimensions. The adaptive mesh refinement is driven by reliable and efficient a posteriori error estimators, and convergence is proven in  $H^2$ -type norms without higher regularity assumptions of the solution. A foundational ingredient in the proof of convergence is the concept of the limit space used to describe the limiting behaviour of the finite element spaces under the adaptive mesh refinement algorithm. We develop a novel approach to the construction and analysis of these nonstandard function spaces via intrinsic characterizations in terms of the distributional derivatives of functions of bounded variation. We provide a detailed theory for the limit spaces, and also some original auxiliary function spaces, that resolves some foundational challenges and that is of independent interest to adaptive nonconforming methods for more general problems. These include Poincare and trace inequalities, a proof of the density of functions with nonvanishing jumps on only finitely many faces of the limit skeleton, symmetry of the Hessians, approximation results by finite element functions and weak convergence results.

# [00674] Modern numerical methods for PDE-constrained optimization and control

**Session Time & Room :**

00674 (1/2) : 5B (Aug.25, 10:40-12:20) @G704

00674 (2/2) : 5C (Aug.25, 13:20-15:00) @G704

**Type :** Proposal of Minisymposium

**Abstract :** Control problems, including optimization problems with PDE constraints, have numerous applications across science and engineering, including chemical processes, mathematical biology, fluid flow control, imaging problems, and mean-field games. Of crucial importance is to develop efficient and robust numerical schemes which can solve mathematical models for such problems and the large-scale optimality systems. This can involve accurate and stable discretization schemes, modern linear algebra to solve systems of equations resulting from such problems, and, increasingly, technologies from parallel computing. This session will cover the state-of-the-art in the design of numerical methods for such problems, arising from a range of scientific applications.

**Organizer(s) :** Dante Kalise, John Pearson

**Classification :** 35Q93, 49M41, 65K10

**Minisymposium Program :**

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00674 (1/2) : 5B @G704 [Chair: Dante Kalise]

## [03637] Recent Developments in Preconditioning for PDE-Constrained Optimization

**Format :** Talk at Waseda University

**Author(s) :** John Pearson (University of Edinburgh)

**Abstract :** In this talk, we survey some recent research into numerical linear algebra for PDE-constrained optimization problems. In particular, we consider preconditioned iterative methods for the robust solution of resulting linear(ized) systems. Having provided some motivation for the construction of effective preconditioners, we briefly summarise some solution strategies devised by the speaker along with collaborators, for time-dependent problems, fluid flow control systems, and multiple saddle-point systems arising from PDE-constrained optimization.

## [01670] GKBO method for global optimization of non-convex high dimensional functions.

**Format :** Talk at Waseda University

**Author(s) :** Federica Ferrarese (University of Verona and Trento)

**Abstract :** The study of numerical methods for global optimization of non-convex high dimensional functions has attracted a lot of attention in recent years. In this talk, a new efficient numerical method for global optimization inspired to classical algorithms will be presented. Different theoretical and numerical results will be shown comparing this algorithm to the classical ones. Finally, further extensions to localized versions of this algorithm, useful to minimize functions with multiple global minima, will be introduced.

## [01649] Online identification and control of PDEs via RL methods

**Format :** Talk at Waseda University

**Author(s) :** Alessandro Alla Michele Palladino (Università degli studi dell'Aquila) Agnese Pacifico (Sapienza, Università di Roma) Andrea Pesare (Bending Spoons)

**Abstract :** In this talk we focus on the control of unknown Partial Differential Equations. Our approach is based on the idea to control and identify on the fly. The control, in this work, is computed using the State Dependent Riccati approach whereas the identification of the model on bayesian linear regression. At each iteration we obtain an estimation of the a-priori unknown coefficients of the PDEs based on the observed data and then we compute the control of the correspondent model. We show by numerical evidence the convergence of the method for infinite horizon problems.

## [03371] A statistical POD approach for feedback boundary optimal control in fluid dynamics

**Format :** Online Talk on Zoom

**Author(s) :** Luca Saluzzi (Scuola Normale Superiore di Pisa) Sergey Dolgov (University of Bath) Dante Kalise (Imperial College London)

**Abstract :** I consider feedback boundary optimal control problems and their reduction by the means of a Statistical Proper Orthogonal Decomposition, method characterized by the introduction of stochastic terms in the model to enrich the knowledge of the Full Order Model and in the collection of optimal trajectories as snapshots. The HJB equation is then solved by a data-driven Tensor Train Cross and applied to the control of the incompressible Navier-Stokes equation in a backward-step domain.

00674 (2/2) : 5C @G704 [Chair: John Pearson]

## [04310] Optimal Control of Some Nonlocal PDEs

**Format :** Talk at Waseda University

**Author(s) :** Roland Herzog (Heidelberg University) Masoumeh Hashemi (Heidelberg University)

**Abstract :** Partial differential equations (PDEs) with nonlocal effects pose various challenges in the analysis as well as the numerical solution. This is all the more true for optimal control problems involving nonlocal PDEs. In this presentation, we will discuss examples of optimal control problems for nonlocal PDEs and exhibit the numerical challenges posed by the associated blocks in the optimality systems.

## [01642] Decentralized strategies for coupled shape and parameter inverse problems

**Format :** Talk at Waseda University

**Author(s) :** Abderrahmane HABBAL (University Cote d'Azur Inria)

**Abstract :** We present a novel family of algorithms framed within game theory setting and dedicated to solve ill-posed inverse problems, where unknown shapes -obstacles or inclusions- or sources are to be reconstructed as well as missing boundary conditions, for steady Stokes fluids.

Some theoretical results and several numerical experiments are provided that corroborate the ability of the approach to tackle harsh problems.

## [04057] Stability-exploiting adaptive finite elements for optimal control

**Format :** Talk at Waseda University

**Author(s) :** Manuel Schaller (Technische Universität Ilmenau)

**Abstract :** Optimal control problems often exhibit a particular stability property which, for time-dependent problems, manifests itself, e.g., by means of a turnpike property. The latter states that optimal solutions to dynamic problems reside close to a particular steady state for the majority of the time. Such a stable behavior can be shown under stabilizability and detectability-like assumptions and in particular also can be shown to hold when the uncontrolled equations are unstable. In this talk, we will show how this stability leads to locality of discretization errors which can be exploited by means of adaptive finite-element methods, leading to a significant reduction in computational expenses, e.g., in a Model Predictive Controller.

# [00675] New trends in (optimal) control theory

**Session Time & Room :**

00675 (1/2) : 4E (Aug.24, 17:40-19:20) @F401

00675 (2/2) : 5B (Aug.25, 10:40-12:20) @F401

**Type :** Proposal of Minisymposium

**Abstract :** The goal of this mini-symposium is to bring together experts in several fields of interest in control and optimal control theory, including controllability, stabilization, and large-time behavior of optimal controls, in order to foster scientific interactions. This mini-symposium also aims to be at the intersection between theoretical issues and applications, notably to machine learning, traffic flow and microswimmers.

**Organizer(s) :** Pierre Lissy, Idriss Mazari

**Classification :** 49K15, 49K20, 93B05, 93B52

**Minisymposium Program :**

00675 (1/2) : 4E @F401 [Chair: Pierre Lissy]

## [01796] Surveillance-evasion games with visibility constraints

**Format :** Talk at Waseda University

**Author(s) :** Carlos Esteve-Yague (University of Cambridge)

**Abstract :** In this talk, I consider a two-player zero-sum game in which the payoff involves the visibility of the players. First, I will present a new analysis of the boundary conditions for the associated Hamilton-Jacobi-Isaacs HJI equation. As we shall see, these boundary conditions turn out to be non-trivial, and the regularity is related to the curvature of the obstacles. Then, using a new notion of visibility, I will introduce suboptimal feedback strategies for the players which can be proven to approximate the optimal feedback given by the solution of the HJI equation. The main advantage of using these suboptimal feedback controls is that they are computationally efficient and are scalable to the case of multiple players.

## [01823] Steering undulatory micro-swimmers in a fluid flow through reinforcement learning

**Format :** Online Talk on Zoom

**Author(s) :** Zakarya El-Khiyati (Université Côte d'Azur, Inria, CNRS, Sophia-Antipolis)Raphaël Chesneaux (Université Côte d'Azur, Inria, CNRS, Sophia-Antipolis)Laetitia Giraldi (Université Côte d'Azur, Inria, CNRS, Sophia-Antipolis)Jérémie Bec (Université Côte d'Azur, Inria, CNRS, Sophia-Antipolis)

**Abstract :** The talk deals with optimal navigation policies for thin, deformable microswimmers, which progress in a viscous fluid flow by propagating a sinusoidal undulation along their slender body. The swimmer has to compete with the drifts, strains, and deformations inflicted by the external flow. Such an intricate situation, where swimming and navigation are tightly bonded, is addressed using various methods of reinforcement learning. A study of the swimming strategies selected set will be provided.

## [02637] Optimization problems under uncertainty

**Format :** Online Talk on Zoom

**Author(s) :** teresa scarinci (Università di Cassino e del Lazio Meridionale)

**Abstract :** The study of models with uncertainty plays an important role in scientific numerical simulations. This class of problems is strongly utilized in engineering, biology, and finance. In this talk, we discuss the importance of including uncertainty in optimal control. Randomness can be utilised to model applications where the data of the problem -- such as the dynamic, the coefficients, or the time delay -- are not known a priori and one knows only statistical information.

00675 (2/2) : 5B @F401 [Chair: Idriss Mazari]

## [01828] Stability of open quantum systems designed by reservoir engineering.

**Format :** Talk at Waseda University

**Author(s) :** Rémi Robin (Laboratoire de Physique de l'école Normale Supérieure, Mines Paris, Inria, CNRS, ENS-PSL, Sorbonne Université, PSL Research University)Pierre Rouchon (Laboratoire de Physique de l'école Normale Supérieure, Mines Paris, Inria, CNRS, ENS-PSL, Sorbonne Université, PSL Research University)Lev-Arcady Sellem (Laboratoire de Physique de l'Ecole Normale Supérieure, Mines Paris, CNRS, ENS-PSL, Inria, Sorbonne Université, PSL Research University, Paris, France)

**Abstract :** Dynamically protected cat-qubits are an open quantum system that stabilizes a finite dimensional subspace of a quantum harmonic oscillator. Such a process is achieved through reservoir engineering, a method of coupling a high-quality cavity with a dissipative one. In this talk, we will present a new generalized LaSalle's invariance principle to prove the long time convergence of this system towards the finite dimensional subspace of interest.

## [01818] Turnpike phenomena in optimal control

**Format :** Talk at Waseda University

**Author(s) :** Roberto Guglielmi (University of Waterloo)

**Abstract :** We provide a characterization of the exponential turnpike property for infinite dimensional generalized linear-quadratic optimal control problems in terms of structural properties of the control system, such as exponential stabilizability and detectability. The proof relies on the analysis of the exponential convergence of solutions to the differential Riccati equations to the algebraic counterpart, and on a necessary condition for exponential stabilizability in terms of a closed range test.

## [02571] Stabilization of traffic flow using fixed bottlenecks

**Format :** Talk at Waseda University

**Author(s) :** Thibault Liard (University of Limoges)

**Abstract :** We study the asymptotic behavior of scalar conservation laws with local side constraints. Our aim is to construct a boundary feedback law, based on a sliding mode procedure, which globally stabilizes G-solutions of scalar conservation laws around a given stationary solutions. To that end, we will extend the notion of generalized characteristics to G-solutions. In the context of vehicular traffic, this leads to control the flow of cars at the tolls of a highway to reach a given target function. Thus, some bottlenecks could be created. Simulations using particle methods will be given to illustrate our results.

## [02530] Optimal Boundary Control for the semilinear Transport Equation under Uncertainty: A Turnpike Result

**Format :** Talk at Waseda University

**Author(s) :** Michael Schuster (FAU Erlangen-Nuremberg)Noboru Sakamoto (Nanzan University Nagoya)

**Abstract :** We show an integral turnpike result for an optimal Dirichlet boundary control problem with a semilinear transport equation in the sense that if the time horizon goes to infinity, then the dynamic optimal control converges to the corresponding steady state optimal control. Further we show that the integral turnpike result also holds if the initial data and/or the source term is uncertain with respect to a random variable

## [00685] Mathematical modeling, simulation and optimization in stroke risk assessment

**Session Time & Room :** 2C (Aug.22, 13:20-15:00) @E820

**Type :** Proposal of Minisymposium

**Abstract :** The aim of the minisymposium is to bring together scientists working on computational and mathematical analysis tools to improve clinical pathways in the exploration, analysis and treatment of stenosis to reduce the risk of ischemic stroke. Topics covered include novel methods for patient specific hemodynamic modeling and simulation, mathematical shape optimization for fluid-structure-interaction, and machine learning approaches. Combining these mathematical approaches with clinical data then allows to complement and improve existing tools for the exploration of risk sites of the corresponding arteries.

**Organizer(s) :** Michael Hinze, Anna Hundertmark

**Classification :** 74F10, 76B75, 76Z05, 92C35, 92C50

**Minisymposium Program :**

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00685 (1/1) : 2C @E820 [Chair: Michael Hinze]

## [03136] Hemodynamic modeling of directional shear risk metrics in the carotid artery

**Format :** Talk at Waseda University

**Author(s) :** Anna Hundertmark (RPTU Kaiserslautern-Landau)Kevin Richter (RPTU Kaiserslautern-Landau)Tristan Probst (RPTU Kaiserslautern-Landau)

**Abstract :** We present a numerical evaluation of hemodynamic risk metrics and their multi-directional behavior in human stenosed carotid artery. In the FSI model considered, the elastic modulus is strain-dependent in agreement with laboratory compliance measurements. We investigate the multidirectional behavior of wall shear stress (WSS) based on specially constructed longitudinal tangent vectors using centerline projection approach. We present the utility of longitudinal WSS evaluation for the detection of opposing or transverse (injurious) WSS in slow flow.

## [03760] Physiological flow simulations for stroke assessemnt and importance of distensiblity

**Format :** Talk at Waseda University

**Author(s) :** Kevin Richter (RPTU Landau)

**Abstract :** In the process of bringing hemodynamic simulations to the clinical forefront we present the creation of a database that can offer guidance in the assessemnt of stroke risks in the carotid bifurcation area. We established a working pipeline for creating CFD simulations for over 100 patient-specific geometries. The importance of realistic boundary conditions are highlighted. To incorporate realistic distensibility of the arterial wall, we compared simulations to *in vivo* experiments.

## [03568] Predicting Stroke Risk with Graph Neural Networks and CFD Simulations

**Format :** Talk at Waseda University

**Author(s) :** Rohit Pochampalli (RPTU Kaiserslautern)Nicolas R. Gauger (RPTU Kaiserslautern)

**Abstract :** We propose a novel approach for predicting stroke risk using graph neural networks (GNNs) and computational fluid dynamics (CFD) simulations. GNNs enable us to capture the complex, nonlinear relationships

between the geometry of the blood vessel and features such as the distribution of shear stresses on the vessel walls, which are known to influence the development of atherosclerosis. Our approach provides new insights into the relationship between blood flow patterns and stroke risk, potentially enabling more personalized prevention and treatment strategies.

### [03834] Shape optimization in applications of blood flows under uncertainties

**Format :** Online Talk on Zoom

**Author(s) :** Georgios Bletsos (Hamburg University of Technology (TUHH))Michael Hinze (Universität Koblenz)Winnifried Wollner (University of Hamburg)Thomas Rung (Hamburg University of Technology (TUHH))

**Abstract :** The goal of this study is to minimize the expected value and standard deviation of blood damaging metrics of biomedical geometries, by updating their shape while considering uncertainties of the flow or the blood modeling.

The robust shape optimization procedure is realized by means of a gradient-descent method. Gradient information is obtained by a hybrid stochastic-deterministic approach or by an adjoint-assisted method in which uncertainty quantification is realized based on the FOSM approach.

## [00686] Higher-order networks for complex systems

**Session Time & Room :**

00686 (1/3) : 3C (Aug.23, 13:20-15:00) @F412

00686 (2/3) : 3D (Aug.23, 15:30-17:10) @F412

00686 (3/3) : 3E (Aug.23, 17:40-19:20) @F412

**Type :** Proposal of Minisymposium

**Abstract :** Complex systems often exhibit emergent phenomena that cannot be understood by studying mere pairwise interactions. Emblematic examples include chemical reaction and molecular biology, where interactions often involve more than just two elements. Nevertheless, most of the mathematical tools of network science have been developed using traditional graphs, which are an explicitly pairwise representation. This mini-symposium will focus on the mathematical objects which are better suited to modelling higher order interactions, such as simplicial complexes and hypergraphs, as well as on the tools that can be used to investigate them.

**Organizer(s) :** Gillian Grindstaff, Heather Harrington, Raffaella Mulas

**Classification :** 55U10, 05C65, 18M35, 92C42

**Minisymposium Program :**

00686 (1/3) : 3C @F412 [Chair: Gillian Grindstaff]

### [02953] Towards mixed volumes of binomial reaction networks

**Format :** Online Talk on Zoom

**Author(s) :** Jane Ivy Coons (University of Oxford)Mark Curiel (University of Hawai'i)Elizabeth Gross (University of Hawai'i)

**Abstract :** Mass action kinetics on a chemical reaction network give rise to a polynomial system of equations. The zeros of this system are the steady states of the network, and its mixed volume is an upper bound on the number of complex steady states. We show that when the steady state ideal is binomial and the conservation laws satisfy a "partitionability" property, the mixed volume can be easily computed as a determinant.

### [02968] A Hypergraph Model of Opinion Dynamics

**Format :** Online Talk on Zoom

**Author(s) :** Abigail Hickok (UCLA)Yacoub Kureh (Industry)Heather Zinn Brooks (Harvey Mudd College)Michelle Feng (Caltech)Mason A. Porter (UCLA)

**Abstract :** Networks encode only pairwise interactions and cannot take into account polyadic interactions. I'll discuss how the incorporation of polyadic interactions (encoded by a hypergraph) changes the qualitative behavior of an opinion dynamics model, which is a model of how people's opinions change with time as they interact. We show that our hypergraph model converges to consensus under a wide range of initial conditions, whereas network models converge to polarization under the same initial conditions.

## [02963] Topological techniques for classification of agent-based tumour-immune model

**Format :** Talk at Waseda University

**Author(s) :** Gillian Grindstaff (University of California, Los Angeles)Jingjie Yang (University of Oxford)Hai Fang (University of Oxford)Jagdeep Dhesi (University of Oxford)Hee Rhang Yoon (Wesleyan University)Joshua A. Bull (University of Oxford)Helen M. Byrne (University of Oxford)Heather A. Harrington (University of Oxford)

**Abstract :** We address the problem of classifying time series of synthetic 2-d spatial data from an agent-based model of tumour growth that includes tumour cells, macrophages, and blood vessels. We implement and compare the predictive power of four topological vectorizations specialized to such cell data: persistence images of Vietoris-Rips and radial filtrations at static time points, and persistence images for zigzag filtrations and persistence vineyards varying in time.

## [02931] Topological methods for spatial data in molecular biology

**Format :** Talk at Waseda University

**Author(s) :** Katherine Benjamin (University of Oxford)

**Abstract :** Single-parameter persistent homology – the flagship tool in topological data analysis – has witnessed a wide range of successful applications in the biological sciences over the last decade. Multiparameter persistent homology is a natural generalisation allowing for higher-order analysis of more complex phenomena including time-varying data. In this talk, we demonstrate some applications of multiparameter persistent homology to spatial data in biology.

00686 (2/3) : 3D @F412 [Chair: Gillian Grindstaff]

## [02955] Clustering and trajectory classification via the Hodge Laplacian

**Format :** Talk at Waseda University

**Author(s) :** Michael Schaub (RWTH Aachen University)

**Abstract :** We present methods to cluster point cloud data and trajectories based on spectral properties of the Hodge Laplacian. Our approach relies on similar ideas as found in spectral embeddings such as Laplacian eigenmaps. However, rather than constructing a single graph to cluster the data, we consider appropriately constructed simplicial complexes, and (a set of) associated Hodge-Laplacians which allow us to leverage a rich set of topological features for classification.

## [02956] Kernel-based independence measures, hypergraphs, and higher-order interactions

**Format :** Talk at Waseda University

**Author(s) :** Mauricio Barahona (Imperial College London)

**Abstract :** This talk will cover the use of kernel-based methods for the detection of higher order interactions and the relationships with formalizations using hypergraphs.

## [02966] Higher-Order Phase Oscillator Networks from Phase Reductions

**Format :** Talk at Waseda University

**Author(s) :** Christian Bick (Vrije Universiteit Amsterdam)

**Abstract :** Synchronization is a fascinating effect of the interaction between coupled oscillatory units and is ubiquitous in biological systems. If the coupling between units is sufficiently weak, phase reductions provide an adequate description of the dynamics. We discuss phase reductions beyond first order that yield phase oscillator networks with higher-order interactions. Specifically, we discuss how the nonpairwise higher-order phase interactions depend on the shape of the limit cycles and the underlying network structure.

## [03193] When do two networks have the same steady state ideal?

**Format :** Talk at Waseda University

**Author(s) :** Mark Curiel (University of Hawaii at Manoa)Elizabeth Gross (University of Hawaii at Manoa)Carlos Munoz (San Jose State University)

**Abstract :** Chemical reaction networks are often used to model biological processes, e.g. cell signaling. Assuming mass action kinetics, a reaction network gives rise to a polynomial system. We consider the ideal generated by these polynomials, called steady-state ideals. Our main results describe three combinatorial operations on the reaction graph that preserve the steady-state ideal. Furthermore, we give combinatorial conditions to identify monomials in a steady-state ideal.

00686 (3/3) : 3E @F412 [Chair: Gillian Grindstaff]

## [02960] Hypergraph representation of topological features in complex systems

**Format :** Talk at Waseda University

**Author(s) :** Agnese Barbensi (The University of Melbourne)

**Abstract :** Understanding how a system's behaviour emerges from its shape and structure is a critical question across modern science. Topological data analysis provides a powerful computational window on this problem. I will present some recent work in which we develop a framework to analyse the behaviour of complex systems via their structures. The proposed method is based on an interpretation of persistent homology summaries with network theoretical tools, combined with statistical and computational techniques.

## [02964] Spectral theory of graphs and hypergraphs

**Format :** Online Talk on Zoom

**Author(s) :** Raffaella Mulas (Vrije Universiteit Amsterdam)

**Abstract :** Spectral graph theory studies the qualitative properties of a graph that can be inferred from the eigenvalues and the eigenvectors of an operator associated with it. It has a long history, and it is widely used in applications. In this talk, we recall the key properties of the graph normalized Laplacian and we generalize it to the case of hypergraphs.

## [02989] Role analysis for higher-order social systems

**Format :** Talk at Waseda University

**Author(s) :** Nina Otter (Queen Mary University of London)

**Abstract :** Social scientists have been using networks to model social systems since at least the 1970s. A social network model is typically a collection of simple graphs, which can be thought of as a multi-relational graph. Studying the roles of actors in the network amounts to studying the semigroup structure of compound relations that arise from the multi-relational graph. These graph models assume a pairwise interaction between social actors. We study ways to extend the analysis of social roles to models that take into account not only pairwise but also higher-order relationships between social actors, such as social simplicial complexes and hypergraphs. A challenge in this process is to define compound higher-order relations with desirable algebraic and topological properties. In this talk I will discuss several ways to address this problem, drawing inspiration from various areas to find an appropriate generalization of composition, including q-analysis, PROPs, and chemical hypergraphs. I will then illustrate how different composition operations capture different types of information in real-world social systems.

The talk is based on joint work in progress, started at the AMS MRC 2022 on Applied Category Theory, jointly with Daniel Cicala, Rachel Hardeman Morrill, Abigail Hickok, Elise McMahon, Nikola Milicevic, Nima Motamed, Emily Roff.

## [02951] Topological Information Retrieval with Dilation-Invariant Bottleneck Comparative Measures

**Format :** Online Talk on Zoom

**Author(s) :** Anthea Monod (Imperial College London)Yueqi Cao (Imperial College London)Athanasios Vlontzos (Advanced Causal Inference (ACI) Lab )Luca Schmidtke (Imperial College London)Bernhard Kainz (Imperial College London)

**Abstract :** Representing elements in a database so that queries may be accurately matched is a central task in information retrieval. This is achieved by embedding the graph of the database into a manifold using a variety of metrics. Persistent homology is able to characterize a database in terms of hierarchy and connectivity. We show that embeddings retaining the database topology coincide topologically with dilation-invariant comparisons, which we propose to address metric distortion on manifolds.

## [00687] Recent advances in deep learning-based inverse and imaging problems

**Session Time & Room :**

00687 (1/3) : 2C (Aug.22, 13:20-15:00) @E605

00687 (2/3) : 2D (Aug.22, 15:30-17:10) @E605

00687 (3/3) : 2E (Aug.22, 17:40-19:20) @E605

**Type :** Proposal of Minisymposium

**Abstract :** The interplay of deep learning with inverse and imaging problems has seen a tremendous progress during the last years producing state-of-the-art results in most tasks. Apart from the availability of large data and the increased computing power, this progress has been mainly facilitated by the development of rigorous theoretical investigations. The purpose of this minisymposium is to bring together experts in data-driven inverse imaging problems who work both in theory and applications. The aim is to stimulate a fruitful knowledge exchange about how mathematical theories can contribute and further develop this field.

**Organizer(s) :** Guozhi Dong, Michael Hintermüller, Kostas Papafitsoros

**Classification :** 65J22, 65K10, 68T07

**Minisymposium Program :**

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00687 (1/3) : 2C @E605 [Chair: Michael Hintermueller]

## [05273] Data-driven parameter optimization for some inverse problems with sparsity-based priors

**Format :** Talk at Waseda University

**Author(s) :** Juan Carlos De los Reyes (MODEMAT)

**Abstract :** In recent years, novel ideas have been applied to several inverse problems in combination with machine learning approaches, to improve the inversion by optimally choosing different parameters of interest. A fruitful approach in this sense is bilevel optimization, where the inverse problems are considered as lower-level constraints, while on the upper-level a loss function based on a training set is used. When confronted with inverse problems with sparsity-based regularizers, however, the bilevel optimization problem structure becomes quite involved to be analyzed, as classical nonlinear or bilevel programming results cannot be directly utilized.

In this talk, I will discuss on a strategy to overcome these difficulties, leading to a reformulation of the bilevel problems as mathematical programs with complementarity constraints. This enables to obtain sharp first-order optimality conditions, but at the price of lifting the problems to a higher dimension. Some ideas on how to reduce the dimension of the problems back will also be presented, together with the different challenges that these problems pose, when dealing with large training sets.

## [03185] Data-driven Joint Inversion for PDE Models

**Format :** Talk at Waseda University

**Author(s) :** Kui Ren (Columbia University)

**Abstract :** The task of simultaneously reconstructing multiple physical coefficients in partial differential equations from observed data is ubiquitous in applications. In this work, we propose an integrated data-driven and model-based iterative reconstruction framework for such joint inversion problems where additional data on the unknown coefficients are supplemented for better reconstructions. Our method couples the supplementary data with the PDE model to make the data-driven modeling process consistent with the model-based reconstruction procedure. We characterize the impact of learning uncertainty on the joint inversion results for two typical model inverse problems. This is based on a joint work with Lu ZHang.

## [02972] A scalable deep learning approach for solving high-dimensional dynamic optimal transport

**Format :** Talk at Waseda University

**Author(s) :** Zuoqiang Shi (Tsinghua University)

**Abstract :** The dynamic formulation of optimal transport has attracted growing interests. In this talk, we propose a deep learning based method to solve the dynamic optimal transport in high dimensional space based on carefully designed representation of the velocity field, the discretization along the characteristics, and the computation of high dimensional integral by Monte Carlo method. Numerical experiments show that our method could give more accurate results in high dimensional cases and has very good scalability.

## [04688] Learning nonlinearities in time-dependent PDEs from data

**Format :** Talk at Waseda University

**Author(s) :** Christian Aarset (University of Göttingen)Martin Holler (University of Graz)Tram Thi Ngoc Nguyen (Max-Planck Institute for Solar System Research, Göttingen)

**Abstract :** We introduce and analyze an all-at-once approach for learning parts of a partial-differential-equation-based model from data. More specifically, we consider the learning of a non-linearity in the model, which acts pointwise on the state, from indirect, noisy measurements. We provide a function-space analysis of the corresponding learning problem and of the resulting PDE with learned components in a general setting. Furthermore, we show numerical experiments that confirm the practical feasibility of the proposed method.

00687 (2/3) : 2D @E605 [Chair: Kostas Papafitsoros]

## [04070] Conductivity imaging using deep neural networks

**Format :** Online Talk on Zoom

**Author(s) :** Bangti Jin (Chinese University of Hong Kong)

**Abstract :** Conductivity imaging from various observational data represents one fundamental task in medical imaging. In this talk, we discuss numerical methods for identifying the conductivity parameters in elliptic PDEs. Commonly, a regularized formulation consists of a data fidelity and a regularizer is employed, and then it is discretized using finite difference method, finite element methods or deep neural networks in practical computation. One key issue is to establish a priori error estimates for the recovered conductivity distribution. In this talk, we discuss our recent findings on using deep neural networks for this class of problems, by effectively utilizing relevant stability results.

## [04396] Model-corrected learned primal-dual models for fast photoacoustic tomography

**Format :** Talk at Waseda University

**Author(s) :** Andreas Hauptmann (University of Oulu)

**Abstract :** Learned iterative reconstructions hold great promise to accelerate tomographic imaging with empirical robustness to model perturbations. Adoption for photoacoustic tomography is hindered by the computational expensive forward model. Computational feasibility can be obtained by the use of fast approximate models, but model errors need to be compensated.

In this talk we discuss conceptual difficulties and present methodological advances for model corrections in learned image reconstructions by embedding the model correction in a learned primal-dual framework.

## [03165] Learning the Regularisation Parameter for Inverse Problems

**Format :** Online Talk on Zoom

**Author(s) :** Sebastian Scott (University of Bath)Matthias Ehrhardt (University of Bath)Silvia Gazzola (University of Bath)

**Abstract :** Solving linear inverse problems via variational regularisation involves the use of unknown regularisation parameters. In order to attain a meaningful reconstruction, these parameters must be carefully chosen. This work will cover bilevel learning, a framework in which one is able to learn appropriate parameter values via a machine learning approach.

## [04247] Lipschitz Training for Adversarially Robust Neural Networks

**Format :** Talk at Waseda University

**Author(s) :** Tim Roith (Friedrich-Alexander-Universität Erlangen-Nürnberg)

**Abstract :** Adversarial examples have revealed the vulnerability of neural networks, making stability and robustness key concerns. To address this, we explore the role of the Lipschitz constant in adversarial machine learning. I will present an algorithm that employs an approximate Lipschitz constant as a regularizer. In each training step, we compute points that aim to maximize a difference quotient. Finally, I will discuss the conceptual limits of methods enforcing a low Lipschitz constant of neural networks.

00687 (3/3) : 2E @E605 [Chair: Guozhi Dong]

## [05448] The Unrolled Dynamics Modeling for Computed Tomography

**Format :** Talk at Waseda University

**Author(s) :** Haimiao Zhang (Beijing Information Science and Technology University)

**Abstract :** Deep learning revolutionized the research paradigm of medical imaging in the last decades. In this talk, I will show our works on combining classical mathematical models in computed tomography (CT) imaging with the modern deep neural network. These new computational imaging techniques give us a broader way of dealing with the medical imaging problem. Furthermore, numerical results demonstrated that the proposed deep models could be generalized to different datasets, scanning geometries, and noise levels.

## [04836] Dictionary learning for an inverse problem in quantitative MRI

**Format :** Talk at Waseda University

**Author(s) :** Guozhi Dong (Central South University)Michael Hintermueller (Weierstrass Institute Berlin)Clemens Sirotenko (WIAS Berlin)

**Abstract :** The field of quantitative Magnetic Resonance Imaging aims at extracting physical tissue parameters from a

sequence of highly under sampled MR images. Mathematically, this can be achieved by estimating a set of unknown parameters in an ODE model. We employ dictionary learning based approaches to regularize the reconstruction process and investigate iterative schemes to solve the resulting non-convex and non-smooth problems for stationarity. Moreover numerical results and open questions are presented.

## [05295] Deformable volumetric Image registration based on unsupervised learning

**Author(s)** : Ahsan Raza Siyal (University of Innsbruck)

**Abstract** : Deformable image registration has found its way into clinical routine, from image-guided adaptive radiotherapy to brain surgery. The traditional methods optimize an objective function independently for each pair of images, which is highly expensive in terms of time and computation. On the other hand, the deformable registration task can be defined as a parametric function and optimize its parameters on available image pairs and the function can be modeled as neural networks which learn the off-set displacement field through unsupervised loss function which contains data similarity term and a regularization term.

## [00690] Computational methods for interfaces in physics and mechanics

**Session Time & Room** :

00690 (1/2) : 2D (Aug.22, 15:30-17:10) @F403

00690 (2/2) : 2E (Aug.22, 17:40-19:20) @F403

**Type** : Proposal of Minisymposium

**Abstract** : This minisymposium gathers analysts interested in the evolution of interfaces, singularities and lower dimensional objects, applied to fracture evolution, inverse problems, or shape optimization, and more. Fracture can be computed by successive minimizations of "free discontinuity" energies, approached with phase-field methods. Evolving or static interfaces, or lower dimensional singularities, can be computed by discretizing geometric measure theoretical objects. Level sets methods can be used to identify defects in conductive media. The speakers address such issues from different point of views or apply similar methods to different problems. This will foster fruitful interaction between the participants and the audience.

**Organizer(s)** : Antonin Chambolle, Blaise Bourdin

**Classification** : 49NXX, 74PXX, 35QXX

**Minisymposium Program** :

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00690 (1/2) : 2D @F403 [Chair: Blaise Bourdin]

## [01367] Computation of free boundary minimal surfaces via extremal Steklov eigenvalue problems

**Format** : Talk at Waseda University

**Author(s)** : Braxton Osting (University of Utah)

**Abstract** : Recently Fraser and Schoen showed that the solution of a certain extremal Steklov eigenvalue problem on a compact surface with boundary can be used to generate a free boundary minimal surface, i.e., a surface contained in the ball that has (i) zero mean curvature and (ii) meets the boundary of the ball orthogonally. In this talk, I'll discuss numerical methods that use this connection to realize free boundary minimal surfaces. Namely, on a compact surface,  $\Sigma$ , with genus  $\gamma$  and  $b$  boundary components, we maximize  $\sigma_j(\Sigma, g) L(\partial\Sigma, g)$  over a class of smooth metrics,  $g$ , where  $\sigma_j(\Sigma, g)$  is the  $j$ -th nonzero Steklov eigenvalue and  $L(\partial\Sigma, g)$  is the length of  $\partial\Sigma$ . Our numerical method involves (i) using conformal uniformization of multiply connected domains to avoid explicit parameterization for the class of metrics, (ii) accurately solving a boundary-weighted Steklov eigenvalue problem in multi-connected domains, and (iii) developing gradient-based optimization methods for this non-smooth eigenvalue optimization problem. Eigenfunctions corresponding to the extremal Steklov eigenvalues are used to generate a free boundary minimal surface. This is joint work with Chiu-Yen Kao and Édouard Oudet.

## [05329] Capturing surfaces using differential forms

**Format :** Talk at Waseda University

**Author(s) :** Stephanie Wang (University of California, San Diego) Albert Chern (University of California, San Diego)

**Abstract :** Exterior calculus has been an important tool in solving numerical PDEs by representing physical quantities as differential forms. In this talk we expand the usage of differential forms to a whole new way of representing curves and surfaces. By doing so we reformulate the classical nonconvex Plateau minimal surface problem into a convex optimization problem, and introduce a new implicit surface representation that permits nonempty boundaries.

## [05617] Nonlocal approximations of anisotropic surface energies on partitions

**Format :** Talk at Waseda University

**Author(s) :** Selim Esedoglu (University of Michigan)

**Abstract :** Nonlocal energies approximating the perimeter of sets and, in the multiphase case, partitions, arise in many settings. In particular, they play an important role in the study of threshold dynamics, an algorithm for multiphase mean curvature motion. Ensuring the convergence of nonlocal energies in the multiphase, anisotropic setting turns out to be tricky but essential for the correct behavior of these numerical methods. I will discuss conditions that guarantee convergence of the anisotropic energies.

## [05463] On some extensions and applications of thresholding schemes

**Format :** Talk at Waseda University

**Author(s) :** Karel Svadlenka (Kyoto University)

**Abstract :** In this talk, I will present two examples of application of suitably modified thresholding schemes, which were originally developed by Merriman, Bence and Osher, and later generalized by Esedoglu and Otto. First example concerns elucidating cell pattern formation in morphogenesis of sensory epithelia, and the other example concerns understanding evolution of anisotropic particles on solid substrate. I will also touch on the mathematical background of the schemes and their numerical implementation.

00690 (2/2) : 2E @F403 [Chair: Antonin Chambolle]

## [05615] Advanced discretization schemes for phase-field fracture

**Format :** Talk at Waseda University

**Author(s) :** Blaise Bourdin (McMaster University) Frédéric Marazzato (Louisiana State University)

**Abstract :** Variational phase-field models of fracture have established themselves as a powerful and efficient computational approach in fracture mechanics. They are based on a regularization of Francfort and Marigo variational energy, where the crack geometry and discontinuous displacements are represented by smooth functions. The most common implementations are based on finite element discretization via continuous finite elements, and a staggered minimization scheme.

In this talk, we present a new discretization scheme where displacements are discretized using discontinuous Lagrange elements and the phase field variable by Crouzeix-Raviart elements. We compare this scheme to the classical continuous Galerkin scheme and highlight how it leads to a better approximation of the fracture energy.

## [01899] Numerical approximation of a viscoelastic Cahn--Hilliard model for tumour growth

**Format :** Talk at Waseda University

**Author(s) :** Dennis Trautwein (University of Regensburg) Harald Garcke (University of Regensburg)

**Abstract :** In this talk, we present a phase-field model for tumour growth, where a diffuse interface is separating a tumour from the surrounding host tissue. In our model, we include biological effects like chemotaxis and transport processes by an internal velocity field. We include viscoelastic effects with a general Oldroyd-B type description with stress relaxation and stress generation by growth. We analyze a numerical approximation of the model with a fully-practical, stable and converging discrete scheme, which preserves the physical properties of the model. Finally, we illustrate properties of solutions with the help of numerical simulations.

## [02809] A second order Cahn Hilliard model for wetting simulation

**Format :** Talk at Waseda University

**Author(s) :** elie bretin (ICJ & INSA Lyon )

**Abstract :** We focus in this talk to the approximation of surface diffusion flow using a Cahn–Hilliard-type model.

We introduce a new second order variational phase field model that associates the classical Cahn-Hilliard energy with two degenerate mobilities. We also propose some simple and efficient numerical schemes to approximate the solutions

and provide 3D numerical simulations of the wetting of a thin tube on various solid supports. This work was done in collaboration with R. Denis, S. Masnou, G. Terii and A. Sengers

## [04707] Finite element minimization of line and surface energies arising in liquid crystals

**Format :** Talk at Waseda University

**Author(s) :** Dominik Stantejsky (McMaster University)

**Abstract :** Originating in the study of defect structures in nematic liquid crystals, we consider the numerical minimization of an energy posed for two-dimensional surfaces  $T$  involving the surface area of  $T$  outside an obstacle  $E$ , as well as the length of the boundary  $\partial T$  and a surface integral over the obstacle surface, generalizing both the obstacle- and Plateau problem. We propose a finite element representation of the energy and minimize using an ADMM algorithm.

## [00696] Scientific Machine Learning for Inverse Problems

**Session Time & Room :**

00696 (1/3) : 4E (Aug.24, 17:40-19:20) @G808

00696 (2/3) : 5B (Aug.25, 10:40-12:20) @G808

00696 (3/3) : 5C (Aug.25, 13:20-15:00) @G808

**Type :** Proposal of Minisymposium

**Abstract :** Inverse problems address learning complex systems from data. They are ubiquitous in various computational science and engineering areas with grand social impacts, e.g., geophysics, climate change, space missions, and health. Solving an inverse problem requires many solves of the forward model and can be challenging for complex and large-scale problems, e.g., those governed by partial differential equations. Recently, the development of scientific machine learning (SciML) has made tremendous progress in overcoming those challenges. This minisymposium covers progress on (i) the methodology development of SciML-based techniques for inverse problems, and (ii) the applications of SciML methods in solving complex inverse problems.

**Organizer(s) :** Jinlong Wu, Peng Chen

**Classification :** 35R30, 68T07

**Minisymposium Program :**

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00696 (1/3) : 4E @G808 [Chair: Jinlong Wu]

## [03211] Learning Stochastic Closures Using Sparsity-Promoting Ensemble Kalman Inversion

**Format :** Talk at Waseda University

**Author(s) :** Jinlong Wu (University of Wisconsin-Madison)Tapio Schneider (California Institute of Technology)Andrew Stuart (California Institute of Technology)

**Abstract :** Closure models are widely used in simulating complex dynamical systems such as turbulence and climate change, for which direct numerical simulation is often too expensive. Although it is almost impossible to perfectly reproduce the true system with closure models, it is often sufficient to correctly reproduce time-averaged statistics. Here we present a sparsity-promoting, derivative-free optimization method to estimate model error from time-averaged statistics. Specifically, we show how sparsity can be imposed as a constraint in ensemble Kalman inversion (EKI), resulting in an iterative quadratic programming problem. We illustrate how this approach can be used to quantify the model error in the closures of dynamical systems. In addition, we demonstrate the merit of introducing stochastic processes to quantify model error for certain systems. We also present the potential of replacing existing closures with purely data-driven closures using the proposed methodology. The results show that the proposed methodology provides a systematic approach to estimating model error in the closures of dynamical systems.

## [03315] Efficient Bayesian Physics Informed Neural Networks for Inverse Problems via Ensemble Kalman Inversion

**Format :** Talk at Waseda University

**Author(s) :** xueyu zhu (Department of Mathematics, University of Iowa)andrew pensoneault (Department of Mathematics, University of Iowa)

**Abstract :** Bayesian Physics Informed Neural Networks (B-PINNs) have gained significant attention for PDE-based inverse problems. Existing inference approaches are either computationally expensive for high-dimensional posterior inference or provide unsatisfactory uncertainty estimates. In this paper, we present a new efficient inference algorithm for B-PINNs that uses Ensemble Kalman Inversion (EKI). We find that our proposed method can achieve inference results with informative uncertainty estimates comparable to Hamiltonian Monte Carlo (HMC)-based B-PINNs with a much reduced computational cost.

## [02563] Neural operator acceleration of PDE-constrained Bayesian inverse problems: Error estimation and correction

**Format :** Talk at Waseda University

**Author(s) :** Lianghao Cao (The University of Texas at Austin)Thomas O'Leary-Roseberry (The University of Texas at Austin)Prashant K. Jha (The University of Texas at Austin)J. Tinsley Oden (The University of Texas at Austin)Omar Ghattas (The University of Texas at Austin)

**Abstract :** In this talk, we explore using neural operators to accelerate infinite-dimensional Bayesian inverse problems (BIPs) governed by nonlinear parametric partial differential equations (PDEs). Neural operators have gained attention in recent years for their ability to approximate nonlinear mappings between function spaces, particularly the parameter-to-solution mappings of PDEs. On the one hand, the computational cost of BIPs can be drastically reduced if the large number of PDE solves required in posterior characterization are replaced with evaluations of trained neural operators. On the other hand, reducing error in the resulting BIP solutions via reducing approximation error of the neural operators in training can be challenging and unreliable.

We provide an a-priori error bound result that implies certain BIPs can be ill-conditioned to the approximation error of neural operators, thus leading to inaccessible accuracy requirements in training. To reliably reduce error of neural operator predictions to be used in BIPs, we consider correcting predictions of a trained neural operator by solving a linear variational problem based on the PDE residual. We show that a trained neural operator with error correction can possibly achieve a quadratic reduction of its approximation error. Finally, we provide a numerical example based on the deformation of hyperelastic materials. We demonstrate that the posterior representation produced using neural operators is greatly and consistently enhanced by the error correction, while still retaining substantial computational speed ups.

## [01533] Ensemble Kalman inversion with dropout in Scientific Machine Learning for Inverse Problems

**Format :** Talk at Waseda University

**Author(s) :** Shuigen Liu (National University of Singapore)Sebastian Reich (Universität Potsdam)Xin Thomson Tong (National University of Singapore)

**Abstract :** Ensemble Kalman inversion (EKI) is an ensemble-based method to solve inverse problems. However, EKI can face difficulties when dealing with high-dimensional problems using a fixed-size ensemble, due to its subspace property where the ensemble always lives in the subspace spanned by the initial ensemble. To address this issue, we propose a novel approach using dropout technique to mitigate the subspace problem. Compared to the conventional localization approach, dropout avoids the complex designs in the localization process. We prove that EKI with dropout converges in the small ensemble settings, and the complexity of the algorithm scales linearly with dimension. Numerical examples demonstrate the effectiveness of our approach.

00696 (2/3) : 5B @G808 [Chair: Peng Chen]

## [03213] Projected variational inference for high-dimensional Bayesian inverse problems

**Format :** Online Talk on Zoom

**Author(s) :** Peng Chen (Georgia Institute of Technology)

**Abstract :** In this talk, I will present a class of transport-based projected variational methods to tackle the computational challenges of the curse of dimensionality and unaffordable evaluation cost for high-dimensional Bayesian inverse problems governed by complex models. We project the high-dimensional parameters to intrinsically low-dimensional data-informed subspaces, and employ transport-based variational methods to push samples drawn from the prior to a projected posterior. Moreover, we employ fast surrogate models to approximate the parameter-to-observable map. I will present error bounds for the projected posterior distribution measured in Kullback--Leibler divergence. Numerical

experiments will be presented to demonstrate the properties of our methods, including improved accuracy, fast convergence with complexity independent of the parameter dimension and the number of samples, strong parallel scalability in processor cores, and weak data scalability in data dimension.

### **[03215] Multifidelity deep neural operators for efficient learning of partial differential equations with application to fast inverse design of nanoscale heat transport**

**Format :** Online Talk on Zoom

**Author(s) :** Lu Lu (University of Pennsylvania)Min Zhu (University of Pennsylvania)

**Abstract :** Deep neural operators can learn operators mapping between infinite-dimensional function spaces via deep neural networks and have become an emerging paradigm of scientific machine learning. However, training neural operators usually requires a large amount of high-fidelity data, which is often difficult to obtain in real engineering problems. Here we address this challenge by using multifidelity learning, i.e., learning from multifidelity data sets. We develop a multifidelity neural operator based on a deep operator network (DeepONet). A multifidelity DeepONet includes two standard DeepONets coupled by residual learning and input augmentation. Multifidelity DeepONet significantly reduces the required amount of high-fidelity data and achieves one order of magnitude smaller error when using the same amount of high-fidelity data. We apply a multifidelity DeepONet to learn the phonon Boltzmann transport equation (BTE), a framework to compute nanoscale heat transport. By combining a trained multifidelity DeepONet with genetic algorithm or topology optimization, we demonstrate a fast solver for the inverse design of BTE problems.

### **[02629] Surrogate modeling for many-body hydrodynamic interactions via graph neural networks**

**Format :** Online Talk on Zoom

**Author(s) :** Wenxiao Pan (University of Wisconsin-Madison)

**Abstract :** This talk presents a new framework, the hydrodynamic interaction graph neural network (HIGNN), for fast simulation of particulate suspensions. It generalizes the state-of-the-art GNN by 1) introducing higher-order structures in graph and 2) reducing the scaling of its prediction cost down to quasi-linear. The HIGNN, once constructed with low training cost, permits fast predictions of the particles' velocities and is transferable across suspensions of different numbers/concentrations of particles subject to any external forcing.

### **[04531] A practical use of neural density estimators for Bayesian experimental design**

**Format :** Online Talk on Zoom

**Author(s) :** Rafael orozco (Georgia Institute of Technology)Mathias Louboutin (Georgia Institute of Technology)Felix Herrmann (Georgia Institute of Technology)

**Abstract :** Neural density estimation is a powerful approach for learning conditional distributions, including Bayesian posteriors in inverse problems. While Bayesian statisticians find these methods promising, some practitioners remain skeptical about their practicality compared to deterministic solutions. We present a practical use case that exploits the posterior entropy minimization properties of conditional neural density estimators to identify optimal experimental designs. By utilizing normalizing flows, we demonstrate our technique's scalability for tackling realistic 2D and 3D inverse problems.

00696 (3/3) : 5C @G808 [Chair: Jinlong Wu]

### **[03214] Solving High-dimensional Inverse Problems with Weak Adversarial Networks**

**Format :** Online Talk on Zoom

**Author(s) :** yaohua zang Yaohua Zang (Zhejiang University)Gang Bao (Zhejiang University)Xiaojing Ye (Georgia State University)Haomin Zhou (Georgia Institute of Technology)

**Abstract :** We present a weak adversarial network approach to numerically solve a class of inverse problems. The weak formulation of PDE in the inverse problem is leveraged with DNNs and induces a minimax problem. Then, the solution can be solved by finding the saddle points in the network parameters. As the parameters are updated, the network gradually approximates the solution of the inverse problem. Numerical experiments demonstrate the promising accuracy and efficiency of this approach.

## [01482] Automatic discovery of low-dimensional dynamics underpinning time-dependent PDEs for inverse problems resolution

**Format :** Online Talk on Zoom

**Author(s) :** Francesco Regazzoni (MOX, Dipartimento di Matematica, Politecnico di Milano)Matteo Salvador (MOX, Dipartimento di Matematica, Politecnico di Milano)Stefano Pagani (MOX, Dipartimento di Matematica, Politecnico di Milano)Luca Dede' (MOX, Dipartimento di Matematica, Politecnico di Milano)Alfio Quarteroni (MOX, Dipartimento di Matematica, Politecnico di Milano)

**Abstract :** We present a novel Machine Learning technique able to learn differential equations that surrogate the solution of space-time-dependent problems. Our method exploits a finite number of latent variables, providing a compact representation of the system state, automatically discovered during training. It allows building, in a fully non-intrusive manner, surrogate models accounting for the dependence on parameters and time-dependent inputs. As such, our method is suitable to accelerate the resolution of inverse problems.

## [00699] Delay and stochastic differential equations in life sciences and engineering

**Session Time & Room :**

00699 (1/4) : 1C (Aug.21, 13:20-15:00) @G404

00699 (2/4) : 1D (Aug.21, 15:30-17:10) @G404

00699 (3/4) : 1E (Aug.21, 17:40-19:20) @G404

00699 (4/4) : 2C (Aug.22, 13:20-15:00) @G404

**Type :** Proposal of Minisymposium

**Abstract :** The purpose of this minisymposium is to bring experts in delay differential and stochastic differential equations

and to discuss recent advancement in the area, as well as applications of dynamical systems to emerging areas of mathematical biology, medicine and engineering. Qualitative behaviour, stability, oscillation will be the focus of theoretical investigations. In theoretical advancement, the focus is on asymptotic behaviour, in particular local and global stability, and its control. The areas of application include population dynamics, modeling brain activity, cancer treatment, and engineering.

**Organizer(s) :** Elena Braverman

**Classification :** 34Kxx, 92D25, 92D30, 92Cxx, 93Exx

**Minisymposium Program :**

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00699 (1/4) : 1C @G404 [Chair: Elena Braverman]

## [04596] Impacts of demographic and environmental stochasticity on population dynamics with cooperative effects

**Format :** Talk at Waseda University

**Author(s) :** Yun Kang (Arizona State University)Tao Feng (Yangzhou University,)Hongjuan Zhou (Arizona State University)Zhipeng Qiu (Nanjing University of Science and Technology)

**Abstract :** This work provides rigorous analysis on stochastic persistence and extinction, ergodicity, and the existence of a nontrivial periodic solution to study the impacts of demographic and environmental stochasticity on population dynamics with component Allee effects. We show that stochasticity may affect population dynamics differently for different strength of Allee effects. Moreover, in the extinction case, demographic and environmental stochasticity can not change the trend of population extinction, but they can delay or promote population extinction.

## [03954] Recent advances in modeling tick-borne dynamics using delay differential equations

**Format :** Talk at Waseda University

**Author(s) :** Jianhong Wu (York University)

**Abstract :** We provide a short survey of recent advances in modeling tick-borne disease transmission dynamics using structured population dynamics models and delay differential equations. Focus will be on those studies relevant to diapause, that

introduces additional delays in the modeling system (and periodic variation of the environment), and on co-feeding transmission route that requires incorporation of individual infestation dynamics into the transmission dynamics at the population level.

## [03402] Delay and Resonance: From Differential Equations to Random Walks

**Format :** Talk at Waseda University

**Author(s) :** Toru Ohira (Graduate School of Mathematics, Nagoya University)

**Abstract :** Various types of oscillatory dynamics are associated with systems with delayed feedback. We present two simple models that take advantage of these oscillations to induce resonating behaviors. The first model is a simple first-order delay differential equation with a time linear coefficient. The other model is a simple stochastic binary bit with delayed feedback. Both models produce transient oscillatory dynamics that can show resonance with the tuned value of the delay.

## [03310] Evolutionary Games with Strategy-Dependent Time Delays

**Format :** Talk at Waseda University

**Author(s) :** Jacek Miękisz (University of Warsaw)

**Abstract :** We present a new behavior of systems with time delays. We show that in differential replicator equations with strategy-dependent time delays, interior stationary states, describing the level of cooperation in evolutionary games of social dilemmas, depend continuously on time delays, they may also disappear or additional states can emerge. A Prisoner's Dilemma model with an asymptotically stable population with just cooperators is presented. We will also discuss some results for finite populations.

00699 (2/4) : 1D @G404 [Chair: John A. D. Appleby]

## [03461] Asymptotic behaviour for nonautonomous Nicholson equations with mixed monotonicities

**Format :** Talk at Waseda University

**Author(s) :** Teresa Faria (Professor/University of Lisbon)

**Abstract :** A general nonautonomous Nicholson equation with multiple pairs of distinct delays is studied. Sufficient conditions for permanence are given, with explicit lower and upper uniform bounds. Imposing an additional condition on the size of some delays, the global attractivity of positive solutions is established. Sharper results are obtained when there exists a positive equilibrium or periodic solution. These results improve on recent literature, due to the generality of the equation and less restrictive constraints.

## [03291] Periodicity and stability in some biological delay models

**Format :** Talk at Waseda University

**Author(s) :** Anatoli F Ivanov (Pennsylvania State University)

**Abstract :** We consider mathematical models of several biological processes which are described by simple form scalar delay differential equations. They include autonomous nonlinear equations as well as equations with periodic coefficients. New criteria for the global asymptotic stability of equilibrium states are proposed. It is proved that the instability of equilibria implies the existence of periodic motions in the models. Explicit examples from applications demonstrating theoretical findings are given.

## [03816] Exponential stability of linear discrete systems with multiple delays

**Format :** Talk at Waseda University

**Author(s) :** Josef Diblík (Brno University of Technology)Josed Diblik (Brno University of Technology)

**Abstract :** The problem of exponential stability of delayed linear discrete systems with multiple delays and with constant matrices is studied. A new degenerated Lyapunov-Krasovskii functional is used to derive sufficient conditions for exponential stability and derive an exponential estimate of the norm of solutions. Though often used in the study of stability, the assumption that the spectral radius of the matrix of linear terms is less than 1 is not applied here.

## [03498] On asymptotic stability of equations and systems with distributed, unbounded and infinite delays

**Format :** Talk at Waseda University

**Author(s) :** Elena Braverman (university of Calgary)Leonid Berezansky (Ben-Gurion University of Negev)

**Abstract :** Many differential equations of mathematical biology assume delayed production process and instantaneous mortality. Introduction of delay can destabilize the unique positive equilibrium and even lead to chaos. However, for

some types of equations and systems, lags in the reproduction term do not change stability properties. Consideration of variable, unbounded and distributed delays emphasizes robustness of this 'absolute stability' property. Influence of an infinite, not just unbounded, delay is also outlined.

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00699 (3/4) : 1E @G404 [Chair: Elena Braverman]

## [04635] Asymptotic classification of forced stochastic systems with memory

**Format :** Talk at Waseda University

**Author(s) :** John A Appleby (Dublin City University)Emmet Lawless (Dublin City University)

**Abstract :** Linear stochastic functional differential equations are among the simplest stochastic systems that possess path-dependence. In recent work, the authors have characterised the asymptotic behaviour, including rates of convergence to equilibria, of solutions of such systems which are not externally forced. In this work, we are able to characterise the asymptotic behaviour of state-independent forcing terms which guarantee specified types of asymptotic rates of decay, growth and fluctuation size, of solutions.

## [04851] Asymptotic analysis of stochastic functional differential equations

**Format :** Talk at Waseda University

**Author(s) :** Emmet Lawless (Dublin City University)John Appleby (Dublin City University)

**Abstract :** In this talk we are concerned with the asymptotic behaviour of the mean square of scalar stochastic functional differential equations with finite delay. We are primarily interested in providing characterisations of various types of mean square stability and discussing the robustness of solutions under perturbations. Additionally, we highlight how our methods of proof can be utilised to make progress in understanding the mean square behaviour of equations of Volterra type.

## [03977] An order-one adaptive scheme for the strong approximation of stochastic systems with jumps.

**Format :** Online Talk on Zoom

**Author(s) :** Conall Kelly (University College Cork)Gabriel Lord (Radboud University)Fandi Sun (Heriot-Watt University)

**Abstract :** Consider a system of SDEs with coefficients that are locally Lipschitz and together satisfy a montone condition. It is known that the explicit Milstein scheme on a uniform mesh fails to converge here.

We construct an adaptive mesh to ensure order-one convergence that reduces the stepsize as solutions approach the boundary of a sphere, and modify it for systems additionally perturbed by Poisson jumps.

We demonstrate our scheme in the modelling of telomere length dynamics.

## [02373] Mathematical Model of Hepatitis B Virus Combination Treatment

**Format :** Online Talk on Zoom

**Author(s) :** Irina Volinsky (Ariel University, Israel)

**Abstract :** HBV has a high mortality rate with respect to other common known diseases. The commonly used cure for chronic HBV cases is the fusion of interferon and analogous nucleoside methods. The addition of IL-2 therapy proposed in this article. This method was validated to be highly effective. This model will take into account the response of the immune system of the patient and will use immune therapy as a support.

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00699 (4/4) : 2C @G404 [Chair: Elena Braverman]

## [04297] The Impact of Time Delays on Synchrony in a Neural Field Model

**Format :** Online Talk on Zoom

**Author(s) :** Sue Ann Campbell (University of Waterloo)Isam Al-Darabsah (Jordan University of Science and Technology)Boantan Rahman (University of Kurdistan Hewler (UKH))Wilten Nicola (University of Calgary)Liang Chen (University of Waterloo)

**Abstract :** We consider a network of Wilson-Cowan nodes with homeostatic adjustment of the inhibitory coupling strength and time delayed, excitatory coupling. Without delay, the system exhibits rich dynamics including oscillations, mixed-mode oscillations, and chaos. We show that Hopf bifurcations induced by the excitatory coupling, the connectivity structure and the delay lead to different phase-locked oscillations: both synchronized and desynchronized. We show that interaction between different Hopf bifurcations can lead to complex solutions, such as intermittent synchronization.

## [03295] Stability analysis of coupled feedback in hematopoiesis

**Format :** Talk at Waseda University

**Author(s) :** Jacques Bélair (Université de Montréal)

**Abstract :** Hematopoiesis, the production of mammalian blood cells, involves an intertwined network of physiological processes, with nonlinear, delayed feedback control mechanisms. We consider a simplified model of the coupled regulation of erythrocytes (red blood cells) and thrombocytes (platelets).

Equilibrium solutions are determined, their stability established and the nature of the oscillations when instability occurs are investigated. The mathematical part of the analysis revolves around a transcendental characteristic equation of second order with two delays.

## [00702] Sequential Decision Making for Optimization, Learning and Search

**Session Time & Room :** 4C (Aug.24, 13:20-15:00) @F412

**Type :** Proposal of Minisymposium

**Abstract :** Key problems such as hyperparameter optimization, model calibration, and inverse/optimal design often involve exploring design spaces to identify desirable designs for one or more objectives of great value and great cost. Intelligently experimenting in this design space is fundamental to gaining valuable, actionable insights in a viable amount of time. In this minisymposium, we will discuss some of the common methodologies for identifying high-performing and optimal designs, including Bayesian and genetic methods, and several exciting applications which motivate the research in this field.

**Organizer(s) :** Michael McCourt

**Classification :** 60G15, 90C26, 62C10

**Minisymposium Program :**

00702 (1/1) : 4C @F412 [Chair: Michael McCourt]

## [04910] Combinatorial 3D Shape Assembly with Sequential Decision-Making Processes

**Format :** Online Talk on Zoom

**Author(s) :** Jungtaek Kim (University of Pittsburgh)

**Abstract :** We require unit primitives, e.g., voxels and points, to create a 3D shape. In particular, if we consider a way to construct a 3D shape with the connectivity of primitives, a problem of 3D shape creation is characterized by sequential and combinatorial properties. By dealing with the sequential and combinatorial properties, we present a method for 3D shape assembly using sequential decision-making processes, i.e., Bayesian optimization and reinforcement learning.

## [05274] Constraint active search as an alternative to optimization

**Format :** Online Talk on Zoom

**Author(s) :** Michael McCourt (Unaffiliated)

**Abstract :** Bayesian optimization is a sample efficient method for identifying high performing configurations of a black box function. This strategy is extremely powerful, but it is often a misguided tool for many practical circumstances -- problems with heavy noise, input/output imprecision, many objectives, discrepancy in cost of objective evalution, or a human-in-the-loop defined objective/preference all are situations where optimization may be the wrong strategy. Here, we discuss the shortcomings of optimization and propose an alternate strategy: the search for a satisfactory set of outcomes, as guided by user-defined performance thresholds. We refer to this as Constraint Active Search, and we present our motivating application as well as some theoretical analysis.

## [05604] Optuna: A Software to Solve Black-box Optimization

**Format :** Online Talk on Zoom

**Author(s) :** Hideaki Imamura (Preferred Networks, Inc)

**Abstract :** Optuna is a software tool for solving black-box optimization problems. It provides a Pythonic interface to describe the search space and objective functions. It supports various algorithms, extensive visualization capabilities, and easy distributed optimization. In this presentation, we will introduce some of the latest features of Optuna and discuss the problem awareness that arises in black-box optimization and its application field, specifically hyperparameter optimization in machine learning.

## [05288] Evolution Strategies: Principles and Practical Issues

**Format :** Online Talk on Zoom

**Author(s) :** Masahiro Nomura (CyberAgent)

**Abstract :** Evolution strategies (ES) is one of the most powerful frameworks for black-box continuous optimization. This talk will describe the design principles behind the empirical success of ES and the representative methods that have often been employed in science and industry. In addition, key issues that may be encountered when using ES in practice will be discussed.

## [00703] Combining machine learning with domain decomposition and multilevel methods

**Session Time & Room :**

00703 (1/2) : 4E (Aug,24, 17:40-19:20) @E812

00703 (2/2) : 5B (Aug,25, 10:40-12:20) @E812

**Type :** Proposal of Minisymposium

**Abstract :** In this minisymposium, recent advances in using machine learning in domain decomposition and multilevel methods will be discussed as well as applying domain decomposition and multilevel techniques to improve different aspects of machine learning algorithms.

**Organizer(s) :** Victorita Dolean, Alexander Heinlein, Axel Klawonn, Rolf Krause

**Classification :** 68T07, 65M55, 65N55, 65K10

**Minisymposium Program :**

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00703 (1/2) : 4E @E812 [Chair: Axel Klawonn]

## [03764] A Domain Decomposition-Based CNN-DNN Architecture for Model Parallel Training

**Format :** Talk at Waseda University

**Author(s) :** Axel Klawonn (University of Cologne)Martin Läser (University of Cologne)Janine Weber (University of Cologne)

**Abstract :** In this talk, a novel domain decomposition-based CNN-DNN (convolutional/deep neural network) architecture is presented that naturally supports a model parallel training strategy and that is loosely inspired by two-level domain decomposition methods. Experimental results for different 2D image classification problems are shown as well as for the classification of 3D computer tomography (CT) scans. The results show that the proposed approach can significantly accelerate the required training time without losing accuracy in most cases.

## [03312] DNN-MG: A Hybrid Neural Network/Finite Element Method

**Format :** Talk at Waseda University

**Author(s) :** Nils Margenberg (Helmut Schmidt University Hamburg)Robert Jendersie (Otto von Guericke University Magdeburg)Christian Lessig (Otto von Guericke University Magdeburg)Thomas Richter (Otto von Guericke University Magdeburg)

**Abstract :** The Deep Neural Network Multigrid Solver (DNN-MG) augments classical finite element simulations in fluid-dynamics by deep neural networks to improve the computational efficiency. To achieve this, it combines a geometric multigrid solver with a DNN that is used when a full resolution of the effects is not feasible or efficient. Our method's efficiency, generalizability, and scalability is demonstrated through applications to 3D benchmark simulations of the Navier-Stokes equations.

## [05268] Combining physics-informed neural networks with multilevel domain decomposition

**Format :** Online Talk on Zoom

**Author(s) :** Alexander Heinlein (Delft University of Technology (TU Delft))Victorita Dolean Maini (University of Strathclyde)Siddhartha Mishra (ETH Zurich)Ben Moseley (ETH Zurich)

**Abstract :** Physics-informed neural networks (PINNs) are a powerful approach for solving problems related to differential equations. However, PINNs often struggle to solve differential equations when they have high frequency and/or multi-scale solutions. In this work, we improve the performance of PINNs in this regime by combining them with domain decomposition. We build on the existing finite basis physics-informed neural networks (FBPINNs) framework and show that adding multilevel modelling to FBPINNs improves their performance.

## [04823] Enhancing training of scientific machine learning applications

**Format :** Talk at Waseda University

**Author(s) :** Alena Kopanicakova (Brown University)

**Abstract :** Scientific machine learning has shown potential in creating efficient surrogates for complex multiscale and multiphysics problems. However, the computational cost of training these surrogates is prohibitively high. We propose a training procedure that utilizes the layer-wise decomposition of a deep neural network in order to construct a nonlinear preconditioner for the standard L-BFGS optimizer. The convergence properties of the novel training method will be analyzed by means of numerical experiments.

00703 (2/2) : 5B @E812

## [04378] A Splitting Approach of Multilevel Optimization with an Application to Physics Informed Neural Networks

**Format :** Talk at Waseda University

**Author(s) :** Valentin Mercier (Université de Toulouse, IRIT, CERFACS, BRLi)Serge Gratton (Université de Toulouse, INP-ENSEEIHT, IRIT,ANITI)Philippe Toint (Namur Center for Complex Systems (naXys), University of Namur)Elisa Riccietti (Université de Lyon, INRIA, EnsL, UCBL, CNRS)

**Abstract :** We propose a multilevel optimization algorithm, based on coordinate-block descent, to solve nonlinear problems while maintaining the advantages of multilevel methods. We demonstrate its effectiveness in solving complex Poisson problems using neural networks (NN) with PINN's method. We address the unique challenges posed by NNs, such as the F-principle, by employing frequency-aware network architectures. Overall, our approach offers a cost-effective solution for solving complex nonlinear optimization problems using neural networks.

## [04367] Improved Accuracy of Physics-Informed Neural Networks Using a Two-Level Training Approach and Lagrange Multipliers

**Format :** Online Talk on Zoom

**Author(s) :** Deok-Kyu Jang (Kyung Hee University)Kyungsoo Kim (Kyung Hee University)Hyea Hyun Kim (Kyung Hee University)

**Abstract :** In this talk, we introduce efficient techniques to enhance accuracy of Physics-Informed Neural Networks (PINNs) for solving second-order elliptic problems. We first present a two-level training approach incorporating a scaling process to capture high-frequency solution components more effectively at the first training stage, and a post-processing residual training step to resolve the remaining low-frequency components. We also introduce a non-overlapping domain decomposition method for PINNs where we employ Lagrange multipliers to enforce suitable interface conditions and boundary conditions so as to improve the solution accuracy further. We demonstrate the effectiveness of our proposed methods through numerical test examples.

# [00704] Numerical Software Libraries Enabling Benefits to Scientific Applications

**Session Time & Room :**

00704 (1/3) : 3D (Aug.23, 15:30-17:10) @E803

00704 (2/3) : 3E (Aug.23, 17:40-19:20) @E803

00704 (3/3) : 4C (Aug.24, 13:20-15:00) @E803

part\_1

**Type :** Proposal of Industrial Minisymposium

**Abstract :** Numerous numerical software libraries have high quality implementations of efficient algorithms and thus facilitate transfer of new algorithms developed in academia into scientific applications, including those in labs and industry. Recently, use of these libraries by labs and industry has significantly increased, and the value of these libraries has been made clear. Several libraries have enabled applications to migrate their simulation codes to the newest exascale systems as well as improve performance and capabilities. We will overview library activities undertaken to ensure value to applications and give examples demonstrating use of new algorithms as well as capability and speed improvements.

**Organizer(s) :** Carol S. Woodward, Ulrike M. Yang

**Classification :** 65Z05, 65Y15, 65Y05

**Minisymposium Program :**

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00704 (1/3) : 3D @E803 [Chair: Dan Martin]

## [01829] The Need of Ecosystems of Numerical Libraries for Applications

**Format :** Talk at Waseda University

**Author(s) :** Ulrike Meier Yang (Lawrence Livermore National Laboratory)

**Abstract :** The emergence of heterogeneous computers with increasingly complex architectures necessitates continuous adaptation of software to take advantage of increased performance potential. Thus, the use of multiple mathematical libraries designed by expert mathematicians and software developers is crucial for application codes. Often, there exist interoperabilities between these libraries. So, as each library is ported to a new computer architecture, it is also important that these libraries continue to work together. This requires a healthy well-designed ecosystem. This talk will discuss the importance of a well-adjusted ecosystem of math libraries and its impact on applications.

## [01773] Factorization based sparse solvers and preconditioners for robust solutions

**Format :** Talk at Waseda University

**Author(s) :** Xiaoye Sherry Li (Lawrence Berkeley National Laboratory)

**Abstract :** Many high fidelity simulation and data analysis involve large-scale multiphysics and multiscale modeling problems that generate highly ill-conditioned and indefinite algebraic equations. The factorization based algorithms are indispensable building blocks in the solver stack to solve these numerically challenging problems. We will highlight how factorizations and low-rank approximate factorizations can be effectively used as standalone direct solvers or as preconditioners for iterative solvers. The focus will be on recent advances in SuperLU and STRUMPACK targeting at exascale machines and applications.

## [01874] Exploring the HPC Frontier with Ginkgo

**Format :** Talk at Waseda University

**Author(s) :** Marcel Koch (KIT)Hartwig Anzt (UTK)Terry Cojean (KIT)

**Abstract :** This talk will give an overview of the Ginkgo library and highlight its features through several integrations. Ginkgo is a modern C++ library composed of numerical linear algebra algorithms which are optimized for multicore processors and Nvidia, AMD, and Intel GPUs. The use of sustainable software development principles allows the rapid development of cutting edge algorithms with high-quality interfaces. Among others, these are used in plasma simulation, cardiac electrophysiology, or CFD.

## [01866] Scalability Study for Planewave DFT Solvers

**Format :** Talk at Waseda University

**Author(s) :** Doru Thom Popovici (LBNL)Mauro del Ben (LBNL)Andrew Canning (LBNL)Osni Marques (LBNL)

**Abstract :** Modern supercomputers vary in compute power and network capabilities. For example, Summit and Frontier make use of GPUs for accelerating computation, while relying on either a fat-tree or dragonfly topology for transferring data between the nodes. On the other hand, Fugaku has thousands of CPUs and uses a six-dimensional torus for communication. In this work, we want to study these differences in the context of scaling the eigenvalue solvers used in planewave DFT calculations. More specifically, we will focus on four algorithms meant to solve a nonlinear eigenvalue problem, namely Conjugate Gradient, RMM-DIIS, Jacobi Davidson and Unconstrained. We will show that for each algorithm different considerations must be taken when parallelizing the computation. We will provide proxy applications for each algorithm, and we will provide a thorough analysis of each code on some of the state-of-the-art supercomputers.

We will emphasize that systematic approaches can be derived to guide the parallelization such that the computation can effectively use the compute and network resources.

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00704 (2/3) : 3E @E803 [Chair: Ulrike Yang]

## [01830] Overview and Application Experiences with SUNDIALS

**Format :** Talk at Waseda University

**Author(s) :** Carol Woodward (Lawrence Livermore National Laboratory)Cody Balos (Lawrence Livermore National Lab)David Gardner (Lawrence Livermore National Laboratory)Daniel Reynolds (Southern Methodist University)

**Abstract :** The SUNDIALS library of time integrators and nonlinear solvers has recently increased its support for large-scale GPU-based systems through new data structures and solver package interfaces. This talk will overview the SUNDIALS packages and recently added capabilities then show results on newly deployed systems. Several applications have taken advantage of these capabilities to improve their time integration performance, and results from a selection of these, including combustion, phase field modeling, and cosmology, will be shown.

Prepared by LLNL under Contract DE-AC52-07NA27344. LLNL-ABS-844590.

## [01626] Experience with Exascale Applications using PETSc/TAO

**Format :** Talk at Waseda University

**Author(s) :** Todd Munson (Argonne National Laboratory)

**Abstract :** In this presentation, we will discuss the extensions of the PETSc/TAO library to support the GPU-based Frontier and Aurora exascale systems and provide some available performance results. We will then provide some perspectives on using PETSc/TAO from an application point of view and conclude with thoughts on future needs to support next generation architectures.

## [01703] On the Design and Performance of Exascale Applications using the Trilinos Solver Framework

**Format :** Talk at Waseda University

**Author(s) :** Roger Pawlowski (Sandia National Laboratories)

**Abstract :** The Trilinos project supplies algorithms and enabling technologies for the solution of large-scale, complex multi-physics engineering and scientific problems on new and emerging high-performance computing architectures. Capabilities include performance portability abstractions, linear solvers, preconditioners, nonlinear solvers, time integration and finite element discretization tools. This talk will focus on recent achievements in developing exascale applications using Trilinos. We will show results from plasma physics simulations for electromagnetic environments and aerodynamics simulations for hypersonic reentry.

## [01837] Paving the road for efficient volume coupling with preCICE

**Format :** Talk at Waseda University

**Author(s) :** David Schneider (University of Stuttgart)Benjamin Uekermann (University of Stuttgart)

**Abstract :** preCICE is an open-source coupling library enabling partitioned multi-physics simulations of separated software packages. It offers methods for data communication, equation coupling, and data mapping. This talk presents new data mapping concepts in preCICE in terms of efficiency and accuracy, which enable users to apply preCICE for large-scale coupling scenarios. The relevance of these new data mapping concepts is demonstrated by showing user-provided example cases.

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00704 (3/3) : 4C @E803 [Chair: Carol Woodward]

## [01915] MFEM: Accelerating Efficient Solution of PDEs at Exascale

**Format :** Talk at Waseda University

**Author(s) :** Tzanio Kolev (Lawrence Livermore National Laboratory)Veselin Dobrev (Lawrence Livermore National Laboratory)John Camier (Lawrence Livermore National Laboratory)Vladimir Tomov (Lawrence Livermore National Laboratory)Julian Andrej (Lawrence Livermore National Laboratory)Will Pazner (Portland State University)

**Abstract :** Efficient exploitation of exascale architectures requires rethinking of the numerical algorithms used in PDE-based simulations to expose fine-grain parallelism and maximize arithmetic intensity. In this talk we present an overview of MFEM ([mfem.org](http://mfem.org)), a library for high-order finite element methods, which powers HPC applications in a wide variety of fields. We review recent advancements in MFEM's discretization solver, and GPU-accelerated algorithms, and demonstrate their impact in several large-scale applications from the US Department of Energy.

## [01650] Exascale-Ready Adaptive Mesh Refinement Applications with AMReX

**Format :** Talk at Waseda University

**Author(s) :** Andrew Myers (LBNL)

**Abstract :** AMReX is a block-structured adaptive mesh refinement library that supports a variety of advanced GPU and CPU architectures. I will describe AMReX and its associated ecosystem of application codes, spanning scientific domains such as astrophysics, plasma physics, wind farm modeling, epidemiology, and more. I will demonstrate how AMReX enables these codes to implement novel modeling capabilities involving a range of computational motifs and to run efficiently on some of the largest supercomputers in the world.

## [01911] Supporting Applications with the Chombo Framework

**Format :** Talk at Waseda University

**Author(s) :** Daniel Francis Martin (Lawrence Berkeley National Laboratory)

**Abstract :** Many scientific and industrial applications solve systems of partial differential equations, and can often benefit from algorithmic strategies like adaptive mesh refinement (*AMR*), higher-order mapped grids, and linear and nonlinear solvers. These are often difficult to implement accurately and efficiently; software frameworks leverage this effort across many applications. We present case studies demonstrating how the modular design of the Chombo software framework supports performant applications, which then feed improved capabilities back into Chombo.

## [01456] Firedrake: Math to Supercomputer

**Format :** Talk at Waseda University

**Author(s) :** Koki Sagiyama (Imperial College London) David A. Ham (Imperial College London)

**Abstract :** Firedrake is an open-source Python package for solving PDEs using finite element methods.

Using the UFL language originally developed for the FEniCS project and other packages in the Firedrake's ecosystem, Firedrake generates efficient finite element codes automatically from the math expressions provided by the users, allowing them to move from one idea to another quickly.

It also provides a transparent access to the linear/nonlinear solvers in the PETSc library.

Here, we will show some recent developments in Firedrake.

# [00707] Theoretical and Numerical Challenges in the Modelling of Fluid Motion

**Session Time & Room :**

00707 (1/3) : 2C (Aug.22, 13:20-15:00) @D102

00707 (2/3) : 2D (Aug.22, 15:30-17:10) @D102

00707 (3/3) : 2E (Aug.22, 17:40-19:20) @D102

**Type :** Proposal of Minisymposium

**Abstract :** The goal of this mini-symposium is to provide a forum for presenting and discussing recent advances in mathematical and numerical modelling of fluid motion. The phenomena under consideration range from small oscillations of fluid droplets to large ocean waves. Topics of interest cover nonlinear waves and solitons in fluids, surface and internal ocean waves, atmospheric flows, as well as fluid dynamics methods for fatigue fracture analysis. In this mini-symposium a holistic approach to fluid dynamics is sought where the problem is studied by modern mathematical methods requiring advanced tools in functional analysis, geometry, PDEs, soliton theory and numerical modeling.

**Organizer(s) :** Rossen Ivanov, Michail Todorov

**Classification :** 76B55, 35Q31, 35Q35, 35Q51, 76B25, 76B25-Solitary waves for incompressible inviscid fluids, 76B55-Internal waves for incompressible inviscid fluids, 35Q31-Euler equations, 35Q35-PDEs in connection with fluid mechanics, 35Q51-Soliton equations

**Minisymposium Program :**

00707 (1/3) : 2C @D102 [Chair: Rossen Ivanov]

## [03903] Paradigm and Long-Time Evolution of Localized Solutions of Wave Systems: Consistency vs Integrability

**Format :** Talk at Waseda University

**Author(s) :** Michail Todorov (Technical University of Sofia)

**Abstract :** Boussinesq's equation was the first model for the propagation of surface waves over shallow inviscid fluid layer. He proved that the balance between the steepening effect of the nonlinearity and the flattening effect of the dispersion maintains the shape of the wave - so termed 'Boussinesq Paradigm.' Apart from the significance for the shallow water flows, this paradigm is very important for understanding the particle-like behavior of nonlinear localized waves. As it should have been expected, most of the physical systems are not fully integrable (even in one spatial dimension) and only a numerical approach can lead to unearthing the pertinent physical mechanisms of the interactions. A different approach to removing the incorrectness is by changing the spatial fourth derivative to a mixed fourth derivative, which resulted into an equation known nowadays as the Regularized Long Wave Equation or Benjamin-Bona-Mahony equation - known as the 'Linear Impedance Relation'. The latter has produced innumerable instances of unphysical results.

## [05180] Modelling of tsunami generated by submarine volcanic eruptions in stratified oceans.

**Format :** Talk at Waseda University

**Author(s) :** Manish kanojia (Trinity College Dublin)

**Abstract :**

We present a novel mathematical model for the generation of tsunamis by submarine volcanic eruptions in stratified oceans. Unlike current models, our model accounts for the complex stratification of the ocean, providing a more accurate representation of the tsunami generation process.

## [05211] Physics-informed neural network for computating steady periodic water waves

**Format :** Talk at Waseda University

**Author(s) :** Lin Chen (Tongji University) Ben Li (Tongji University) Chenyi Luo (ETH Zurich)

**Abstract :** We investigate full-field recovery and computation of rotational flow under nonlinear periodic water waves using physics-informed neural networks (PINNs). Flow characteristics beneath water waves are of interest in various disciplines, e.g., for hydraulic loading analysis. In ocean or water tunnel tests, wave heights, flow velocity, and pressure data are often collected at specific points. It is not feasible to measure the flow with very high spatial resolution, particularly for water waves with a wavelength of over 100 m in practice. Therefore, we develop PINNs for flow recovery taking multiple types of measurement data into account and with the Euler equation governing rotational flow embedded. High-fidelity datasets are obtained using the numerical continuation method which is able to solve nonlinear waves with limiting wave height. Different PINN architectures are proposed and compared based on the numerically computed datasets. Influences of the wave height, vorticity, the volume of datasets, and hyperparameters are discussed in detail.

## [01814] Pressure distribution on seawalls due to wave effects

**Format :** Talk at Waseda University

**Author(s) :** Paul Suman (Indian Institute of Engineering Science and Technology, Shibpur) Aparna Dey Ghosh (Indian Institute of Engineering Science and Technology, Shibpur) Biswajit Basu (Trinity College Dublin)

**Abstract :** A numerical approach to obtain wave forces on seawalls is proposed using Bernoulli's equation. The nonlinear formulation computes horizontal and vertical velocities, and pressure distribution along the depth, without any restriction on wave height. Forces are obtained on the seawall for nonbreaking travelling waves. The wave force increases for waves of longer time periods. The existing guidelines are found to overestimate the wave forces as compared to the forces obtained from the proposed nonlinear formulation.

## [02962] Internal waves, Coriolis force and undercurrents

**Format :** Talk at Waseda University

**Author(s) :** Rossen I. Ivanov (Technological University Dublin) David J. Henry (University College Cork)

**Abstract :** We study the linear and nonlinear differential equations modelling the interacting surface and internal waves of two fluid layers with different densities over a flat bed. Other effects such as underlying currents and Coriolis force are also included. We use the Hamiltonian formulation for the nonlinear governing equations that is adequate for structure-preserving perturbations, at the linear and at the nonlinear level.

Specific weakly nonlinear long-wave regimes are structure-enhancing and the dynamics is described by integrable Hamiltonian equations. Consequently, integrable models and their soliton solutions will be presented.

## [05173] On three dimensional models of equatorial ocean flows

**Format :** Talk at Waseda University

**Author(s) :** BISWAJIT BASU (Trinity College Dublin)

**Abstract :** A recently developed three dimensional model of equatorial ocean flow is presented in this paper. The model is inspired by the work of Constantin and Johnson and provides some explicit solution of velocity fields. The effect of density variation is discussed alongwith the influence of undercurrent. Some additional insights are provided based on conservation of potential vorticity.

## [03835] Eddy viscosities and ageostrophic wind-speed profiles

**Format :** Online Talk on Zoom

**Author(s) :** Tony Lyons (South East Technological University)

**Abstract :** Wind speed profiles in the Ekman layer are used to deduce corresponding variable eddy coefficients. These eddy coefficients are parameterized in terms of a deflection angle, the geostrophic wind speed, and the transfer rate of horizontal momentum in the vertical direction. The classical Ekman flow has deflection angle  $45^\circ$ , while incorporating variable eddy coefficients changes this deflection angle. This deviation of deflection angle is used to estimate the depth of the Ekman layer.

00707 (3/3) : 2E @D102

## [00708] Computational medicine of the heart: towards cardiac digital twins

**Session Time & Room :**

00708 (1/3) : 1C (Aug.21, 13:20-15:00) @E708

00708 (2/3) : 1D (Aug.21, 15:30-17:10) @E708

00708 (3/3) : 1E (Aug.21, 17:40-19:20) @E708

**Type :** Proposal of Minisymposium

**Abstract :** Computational cardiology is an emerging field that exploits Mathematics, Engineering, and Computational Science to develop quantitative approaches for understanding the mechanisms of cardiac physiology, for enhancing the diagnosis of pathologies, and for improving their clinical treatment. This minisymposium aims at gathering mathematicians, engineers, and more generally researchers working on mathematical and numerical modelling of the human heart. Topics may include, but are not limited to, coupled cardiac modelling, numerical methods, translational medicine, Scientific Computing, Scientific Machine Learning, and large-scale computing. The overarching aim is the construction of Cardiac Digital Twins.

**Organizer(s) :** Luca Dede', Alfio Quarteroni

**Classification :** 65Mxx, 65Nxx, 68Txx

**Minisymposium Program :**

00708 (1/3) : 1C @E708 [Chair: Alfio Quarteroni]

## [04495] Multiphysics, multiscale, and computational models for simulating the cardiac function

**Format :** Talk at Waseda University

**Author(s) :** Luca Dede' (Politecnico di Milano)

**Abstract :** We present our novel 4-chambers model of the human heart. We couple state-of-the art models of electrophysiology, mechanical activation, passive mechanical response, and blood circulation, leading to a coupled electromechanical problem. Our multiscale model accounts for microscopic active force generation that exploits Machine Learning algorithms. We numerically solve the model in the HPC framework. We also present a Machine Learning method for real-time numerical simulations that allows efficient construction of cardiac digital twins.

## [03710] Virtual Populations of Heart Chimaeras: Generative Compositional Learning from Datasets of Datasets

**Format :** Talk at Waseda University

**Author(s) :** Alejandro Federico Frangi (University of Leeds)Haoran Dou (University of Leeds)Seppo Virtanen (University of Leeds)Nishant Ravikumar (University of Leeds)Zeike Taylor (University of Leeds)

**Abstract :** Virtual populations capturing sufficient anatomical variability while remaining plausible are central to conducting in-silico trials of medical devices. Unfortunately, not all anatomical information is available from a single data sample or modality given a population. Instead, data with missing/partially overlapping anatomical information is often available from independent data samples and/or modalities. We introduce a generative anatomical model capable of learning complex anatomical structures from datasets of unpaired datasets and synthesising anatomical assemblies coined virtual chimaeras.

## [03238] The role of the Eikonal model in personalized cardiac modeling from parameter acquisition to arrhythmia simulations

**Format :** Talk at Waseda University

**Author(s) :** Cristian Alberto Barrios Espinosa (Karlsruhe Institute of Technology (KIT))Jorge Sanchez Arciniegas (Valencia Polytechnic University )Laura Unger (Karlsruhe Institute of Technology (KIT))Marie Houillon (Karlsruhe Institute of Technology (KIT))Armin Luik (Städtisches Klinikum Karlsruhe)Axel Loewe (Karlsruhe Institute of Technology (KIT))

**Abstract :** The Eikonal model is widely used to simulate wave propagation in different fields, including cardiac modeling. A modified version of the Eikonal model can help to customize model parameters, like conduction velocity accounting for anisotropic propagation. Moreover, the modified Eikonal model can be used to simulate arrhythmia by allowing for reactivation, overcoming challenges of the fast iterative method. Finally, we show applications of the enhanced Eikonal models as a valuable tool for cardiac research applications.

## [03521] An anisotropic eikonal model for cardiac repolarization and arrhythmias

**Format :** Talk at Waseda University

**Author(s) :** Simone Pezzuto (Università di Trento)Lia Gander (Università della Svizzera italiana)Rolf Krause (Università della Svizzera italiana)Martin Weiser (Zuse Institute Berlin)Francisco Sahli Costabal (Pontificia Universidad Católica de Chile)

**Abstract :** State-of-the-art computational models of cardiac electrophysiology are computationally expensive. Their clinical applicability is, therefore, limited. In the talk, we will present a lightweight eikonal approximation for real-time simulation of cardiac arrhythmias on a desktop computer. We provide several numerical tests and comparisons, including atrial fibrillation, ventricular tachycardia, and with fibrosis. Finally, we consider the problem of estimating the inducibility of fibrillation with a multi-fidelity framework by combining the eikonal approach with the high-fidelity model.

00708 (2/3) : 1D @E708 [Chair: Alfio Quarteroni]

## [05281] Computational Models of Cardiac Electro-mechanical Function – Closing the Gaps between Virtual and Physical Reality

**Format :** Talk at Waseda University

**Author(s) :** Gernot Plank (Medical University of Graz)

**Abstract :** A fundamental concern hampering a broader adoption of digital twins in cardiology application is the lack of correspondence between the physiology of a virtual heart and the physical reality. We report on our latest advances addressing these issues. Real-time enabled whole heart electrophysiology as well as computationally efficient whole

heart multi-physics models of cardiac electro-mechanics will be discussed, along with techniques for automated patient-specific model calibration.

## [04706] Scaling cardiac digital twins for population-based studies

**Format :** Talk at Waseda University

**Author(s) :** Shuang Qian (King's College London)Devran Ugurlu (King's College London)Elliot Fairweather (King's College London)Marina Strocchi (King's College London)Laura dal toso (King's College London)Yu Deng (King's College London)Alistair Young (King's College London)Martin Bishop (King's College London)Pablo Lamata (King's College London)Steven Niederer (King's College London)

**Abstract :** Cardiac digital twins, provide a physics and physiology-constrained framework, enabling personalised diagnosis and tailored therapies for individual patients. However, building patient-specific digital twins at scale remains challenging. This talk presents an open-sourced automatic pipeline of generating finite element biventricular heart models from CMRs in the UK biobank. Using this pipeline, each digital twin can be created in only 8 mins on a standard desktop, compatible with clinical time scales and also enabling large scale virtual population-based studies.

## [04251] A Local Space-Time Adaptive Scheme to Simulate Cardiac Electrophysiology

**Format :** Talk at Waseda University

**Author(s) :** Dennis Ogiermann (Ruhr University Bochum, Chair of Continuum Mechanics)Luigi E. Perotti (University of Central Florida, Mechanical and Aerospace Engineering Department, Computational Biomechanics Lab)Daniel Balzani (Ruhr University Bochum, Chair of Continuum Mechanics)

**Abstract :** Cardiac electrophysiology simulations are often based on the monodomain model, which is characterized by traveling waves with a steep localized wavefront and slow changes in the remaining domain. This aspect renders schemes based on uniform spatial and temporal discretization expensive.

We present a numerical scheme that exploits the localized nature of the rapidly changing wavefront by combining discontinuous Galerkin on an adaptive mesh for the spatial discretization with an elementwise explicit local time stepping.

## [03847] Parallel Performance of Robust and Scalable Multilevel Preconditioners in Cardiac Electrophysiology

**Format :** Talk at Waseda University

**Author(s) :** Edoardo Centofanti (Università degli Studi di Pavia)

**Abstract :** The EMI (Extracellular space, cell Membrane and Intracellular space) model is among the first models for describing the electrical activity of the heart at a cellular level. The resulting system of equations allows discontinuities of potentials between boundaries as well as particular distributions of ion charges on the cellular membranes. In this talk, we will study the performances of different multigrid and multilevel solvers for the solution of such systems both on CPU and GPU architectures.

00708 (3/3) : 1E @E708 [Chair: Luca Dede']

## [04140] Cardiac hemodynamics simulations with fluid-structure interaction and reduced valve modeling

**Format :** Talk at Waseda University

**Author(s) :** Miguel A. Fernández (Inria)Oscar Ruz (Inria)Jérôme Diaz (Inria)Marina Vidrascu (Inria)Philippe Moireau (Inria)Dominique Chapelle (Inria)

**Abstract :** The development of efficient physiological simulations of the complete FSI phenomena involved in the heart is a challenging problem. We investigate an hybrid approach which combines FSI in the myocardium with a reduced modeling of the valves. A loosely coupled treatment of the interface coupling facilitates the treatment of the isovolumetric phases. The benefits of the proposed approach are investigated and compared with kinematic uncoupling in simulations of the left heart hemodynamics.

## [03773] Parametric Fluid-structure interaction solvers for haemodynamics

**Format :** Talk at Waseda University

**Author(s) :** Damiano Lombardi (Inria Paris)Sébastien Riffaud (Inria Paris)Miguel A. Fernández (Inria Paris)

**Abstract :** Data assimilation and uncertainty quantification are essential tasks in numerous realistic applications.

They involve a prohibitive computational burden. The goal of the present work is to propose and investigate efficient parametric solvers for Partial Differential Equations describing fluid-structure interaction. The solvers consider parameters as extra variables and enable applications such as parameter estimation and uncertainty quantification.

Several formulations will be discussed and numerical experiments will be presented to assess the properties of the methods.

## [04521] Towards developing high-speed cardiac mechanics simulations using a neural network finite element approach

**Format :** Online Talk on Zoom

**Author(s) :** Michael S Sacks (University of Texas at Austin) Shruti Motiwale (University of Texas at Austin)

**Abstract :** We have developed a neural network finite element (NNFE) approach for cardiac simulations, which is a physics-based method using a neural network to solve the parametric map and finite elements to define the problem domain. Cardiac simulations were performed to predict the P-V responses of a simulated left ventricle, accounting for active contraction and transmural fiber distributions. Results demonstrate the first application of the NNFE approach at the organ level within clinically relevant timeframes.

## [05099] Modeling Cardiac Fluid-Structure Interaction in the Human Heart

**Format :** Online Talk on Zoom

**Author(s) :** Marshall Davey (University of North Carolina at Chapel Hill) Charles Puelz (Baylor College of Medicine) Simone Rossi (University of North Carolina at Chapel Hill) Margaret Anne Smith (University of North Carolina at Chapel Hill) David R. Wells (University of North Carolina at Chapel Hill) Boyce E. Griffith (University of North Carolina at Chapel Hill)

**Abstract :** Cardiac fluid-structure fundamentally involves interactions between complex blood flows and the structural deformations of the muscular heart walls and the thin, flexible valve leaflets. This talk will detail methods and models for simulating cardiac fluid-structure interaction in a comprehensive, image-based model of the human heart. The talk will highlight key methodological approaches to developing the model along with simulation results demonstrating its ability to generate physiologic outputs, including realistic pressure-volume loops.

# [00710] Gender Equality in Mathematics: A Global Perspective

**Session Time & Room :**

00710 (1/2) : 3C (Aug.23, 13:20-15:00) @G302

00710 (2/2) : 3D (Aug.23, 15:30-17:10) @G302

**Type :** Proposal of Industrial Minisymposium

**Abstract :** In the last decade, the fields of mathematics and applied mathematics have increasingly recognized the highly creative contributions by women. However, there still remains a significant gap in the percentage of women in these fields, and barriers to achievement by women persist, especially in developing countries. The Gender Gap in Science project was executed to accumulate data on this gap and to provide recommendations on how to reduce and remove barriers to women. Speakers will discuss the gender gap in mathematics globally and overview challenges and activities to address the gap. The sessions will conclude with a moderated panel discussion.

**Organizer(s) :** Carol S. Woodward, Maria Esteban, GuiYing Yan

**Classification :** 01A80

**Minisymposium Program :**

00710 (1/2) : 3C @G302 [Chair: Carol Woodward]

## [01733] Lessons on the global mathematical community from the 'Gender Gap in Science' global survey.

**Format :** Talk at Waseda University

**Author(s) :** Maria J. Esteban (CNRS and University Paris-Dauphine)

**Abstract :** This talk will present the 'Gender Gap in Science' project and more specifically the global survey that was carried out in order to better understand the gender gap in Academia, continent by continent, field by field.

This will be completed with the description of the main results concerning Mathematics and Applied Mathematics in contrast with other scientific fields.

## [02137] The African perspective about the Gender Gap in Science

**Format :** Talk at Waseda University

**Author(s) :** Sophie Dabo (INRIA- University of Lille) Maria J. Esteban (CNRS and University Paris-Dauphine) Colette Guilloté (University Paris Est Creteil) Marie-Françoise Ouedraogo (University Joseph ki\_zeRBO) Marie-Françoise Roy (University of Rennes 1)

**Abstract :** In this talk, we aim to understand the results of the "Gender Gap in Science survey (2017-2019)" for African continent. We analyze in detail the gender gap in Science among scientists who are working in Africa, but also compare those

results with the rest of the world, in particular to see how economical and cultural differences can affect the gender gap among scientists.

Note that that survey addresses several aspects that often are not measured on bibliographic metadata such as work-life balance, family support, access to resources and sexual harassment.

It is important to note also that even if the number of answers was important both in Africa as elsewhere, these numbers are small compared to the whole population of scientists. Also it is necessary to understand that the answers are often subjective because they do not correspond to questions for which the answers are quantifiable, but to how people feel about some particular topic. All this to say that what we are going to state in this talk, is just an image that probably reflects the reality, but that has to be taken with a grain of attention.

## [02048] gender diversity in Japanese concept

**Format :** Talk at Waseda University

**Author(s) :** Motoko KOTANI (Tohoku University)

**Abstract :** Japan is quite behind in gender equality and inclusive perspective. The progress is slow but steady. I would like to present the current situation and actions in Japan, in science in general, and in mathematics.

## [02437] What we can do with Asian-Oceanian Women in Mathematics

**Format :** Talk at Waseda University

**Author(s) :** Yukari Ito (The University of Tokyo)

**Abstract :** Asian-Oceanian Women in Mathematics (AOWM), the continental organization for women in mathematics in Asia and Oceania was established on August 1, 2022. There are more than 200 founding members from 18 Asian and Oceanian countries. We will have the first Inaugural meeting of AOWM in India and hybrid from 24th to 28th April 2023. I will talk about the report of the meeting and what we can do with AOWM.

00710 (2/2) : 3D @G302 [Chair: Maria Esteban]

## [02658] Women in mathematics: an experience report and some facts about the European situation

**Format :** Online Talk on Zoom

**Author(s) :** Carola-Bibiane Schönlieb (University of Cambridge)

**Abstract :** In this talk I will discuss some facts about the situation of female mathematicians in Europe, provide an introduction to the European Women in Mathematics (EWM) association, and give a personal account on women and mathematics in our society.

## [03111] Challenges for US Women in Math and the Activities of the AWM

**Format :** Online Talk on Zoom

**Author(s) :** Talitha Washington (Association for Women in Mathematics)

**Abstract :** While there have been many strides in getting more women into the mathematical sciences, the percentage of women receiving doctorates in mathematics has been decreasing. The complexities of the intersectionality of gender, race, and ethnicity warrant more diverse approaches. The purpose of the Association for Women in Mathematics (AWM) is to create a community where women can thrive. This presentation will share how AWM's activities promote equitable opportunity for women and others of marginalized genders.

## [01795] The Standing Committee for Gender Equality in Science

**Format :** Talk at Waseda University

**Author(s) :** Carol Woodward (Lawrence Livermore National Laboratory)

**Abstract :** Several unions in the International Science Council formed the Standing Committee for Gender Equality in Science (SCGES) in 2020 with the goal of promoting gender equality across all science disciplines. This talk will introduce the SCGES and discuss its activities, including delivery of a webinar series, an annual reporting activity to help share activities among participants, participation in the Global Women's Breakfast, and the release of a statement on

part\_1

gender equality in times of COVID-19.  
LLNL-ABS-844495.

## [02912] Panel Discussion on Gender Equality

**Format :** Talk at Waseda University

**Author(s) :** Carol Woodward (Lawrence Livermore National Laboratory) Maria J. Esteban (CNRS and University Paris-Dauphine) GuiYing Yan (Shandong University)

**Abstract :** In this session, we will have a panel discussion with speakers from our minisymposium discussing the state of gender equality in science and mathematics specifically.

## [00711] Recent Advances in Optimal control and optimization

**Session Time & Room :**

00711 (1/2) : 1C (Aug.21, 13:20-15:00) @F401

00711 (2/2) : 1D (Aug.21, 15:30-17:10) @F401

**Type :** Proposal of Minisymposium

**Abstract :** In this minisymposium we discuss the recent developments in control and optimization.

We analyze solutions to PDE in a general framework and develop a new control and optimization methods and theoretic analysis.

The control PDE analysis includes the constrained stochastic Nash game, optimal control problems in metric spaces and optimal control of poroelastic systems and frequency dependent Hautus tests for controllability. We apply our methods to specific examples in biomedicine, population dynamics and Economics. Also, we develop a new theoretic framework for optimal control and optimization based on Rockafellar's perturbation theory to analyze and solve general nonsmooth convex minimization and monotone inclusion problems.

**Organizer(s) :** Kazufumi Ito

**Classification :** 49J52, 49J55, 49J30, 49J20, 35A01

**Minisymposium Program :**

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00711 (1/2) : 1C @F401

## [02838] PDE Constrained Optimization with Non-smooth Learning Informed Structures

**Author(s) :** Michael Hintermueller (Weierstrass Institute Berlin)

**Abstract :** A class of optimization problems subject to PDEs with components resulting from ReLU-based neural network models is studied analytically and numerically. Concerning the analysis it is shown that direct classical smoothing of the non-smooth structures leads to issues concerning the existence of solutions. Further, for the non-smooth setting stationarity conditions are derived and used numerically. With respect to the numerical solution, a bundle-free minimization algorithm relying on possible smoothing on the level of directional derivatives is introduced and analyzed, and a brief report on computational tests is provided.

## [03725] Some optimal control problems in metric spaces

**Author(s) :** Hasnaa Zidani (INSA Rouen Normandie) Othmane Jerhaoui (INSA Rouen Normandie) Averil Prost (INSA Rouen Normandie)

**Abstract :** In this talk, we will discuss some optimal control problems in metric spaces (e.g. stratified systems, centralized control problems in Wasserstein space). We are mainly interested in the characterisation of the value function as viscosity solution of an adequate Hamilton-Jacobi (HJ) equation. For this, we introduce a notion of viscosity solutions for HJ equations in some metric spaces. This notion is based on test functions that are directionally differentiable and can be represented as a difference of two semi-convex functions. Under mild assumptions on the Hamiltonian and on the metric space, we can derive the main properties of viscosity theory: the comparison principle and Perron's method.

## [03787] Exact controllability for systems describing plate vibrations. A perturbation approach.

**Author(s)** : Marius Tucsnak (University of Bordeaux)

**Abstract** : The aim of this talk is to describe new exact controllability properties of systems described by perturbations of the classical Kirchhoff plate equation. We first consider systems described by an abstract plate equation with a bounded control operator. The generator of these systems is perturbed by bounded operators which are not necessarily compact, thus not falling in the range of application of compactness-uniqueness arguments. Our first main result is abstract and can be informally stated as follows: if the system described by the corresponding unperturbed abstract wave equation, with the same control operator, is exactly controllable (in some time), then the considered perturbed plate system is exactly controllable in arbitrarily small time. The employed methodology is based, in particular, on frequency-dependent Hautus type tests for systems with skew-adjoint operators.

When applied to systems described by the classical Kirchhoff equations, our abstract results, combined with some elliptic Carleman-type estimates, yield exact controllability in arbitrarily small time, provided that the system described by the wave equation in the same spatial domain and with the same control operator is exactly controllable. The same abstract results can be used to prove the exact controllability of the system obtained by linearizing the von K'arm'an plate equation around a real analytic stationary state. This leads, via a fixed-point method, to our second main result: the nonlinear system described by the von K'arm'an plate equations is locally exactly controllable around any stationary state defined by a real analytic function.

## [03789] A Perturbation Framework for Convex Minimization with Nonlinear Compositions

**Author(s)** : Luis Briceño-Arias (Universidad Técnica Federico Santa María)Patrick L. Combettes (North Carolina State University)

**Abstract** : We introduce a framework based on Rockafellar's perturbation theory to analyze and solve general nonsmooth convex minimization and monotone inclusion problems involving nonlinearly composed functions as well as linear compositions.

00711 (2/2) : 1D @F401

## [03864] Analysis and Control in Poroelastic Systems

**Author(s)** : Lorena Bociu (NC State University)

**Abstract** : We answer questions related to tissue biomechanics via wellposedness, sensitivity analysis, and optimal control problems for fluid flows through deformable porous media. These results are relevant for many applications in biology, medicine and bio-engineering. We focus on the local description of the problem, which involves implicit, degenerate, nonlinear poroelastic systems, as well as scenarios where the global features of the problem are accounted for through a multi-scale coupling with a lumped hydraulic circuit.

# [00715] Recent Trends in Market Design

**Session Time & Room** :

00715 (1/3) : 2C (Aug.22, 13:20-15:00) @D505

00715 (2/3) : 2D (Aug.22, 15:30-17:10) @D505

00715 (3/3) : 2E (Aug.22, 17:40-19:20) @D505

**Type** : Proposal of Minisymposium

**Abstract** : Market design, also known as mechanism design, is a practical application of game theory, whose purpose is to develop decision making rules under which each individual has an incentive to take a desirable action in an equilibrium. In recent years, the research of market design has attracted the attention of researchers in various research fields, including mathematics, economics, computer science, biology, politics, psychology, etc. We have nine prospective researches in this minisymposium as invited speakers, who give us state-of-the-art of the theory and applications of market design.

**Organizer(s)** : Ayumi Igarashi, Shunya Noda, Taiki Todo

**Classification** : 91B03, 90B99, 68W01, 91B14, 91A68

**Minisymposium Program** :

## [01261] Fair division algorithms for house chores

**Author(s)** : Ayumi Igarashi (The University of Tokyo)

**Abstract** : Couples often encounter the challenge of sharing house chores. This raises the fundamental question of how to divide chores. In this paper, we present a new application for a fair division of household chores. Our platform, called Kajibuntan, allows couples to specify the set of chores to be shared, their preferences over them, and the current allocation. Our tool visualizes the current allocation and makes proposals according to their preferences based on the theory of fair division. The goal of our tool is to provide a systematic and transparent system to divide household chores and help creating harmony in the home.

## [01327] Mechanism Design with Uncertainty

**Author(s)** : Taiki Todo (Kyushu University)

**Abstract** : My research is summarized as mechanism design with uncertainty. Traditional mechanism design focuses on static environments where all the (possibly probabilistic) information about the agents are observable by the mechanism designer. In practice, however, it is possible that the set of participating agents and/or some of their actions are not observable a priori. We therefore focused on various kinds of uncertainty in mechanism design and developed/analyzed several market mechanisms that incentivize agents to behave in a sincere way.

## [01399] Best of Both Worlds in Fair Division

**Author(s)** : Rohit Vaish (IIT Delhi)

**Abstract** : Traditional approaches for fair allocation of indivisible resources focus either on randomized allocations that are fair in expectation or deterministic allocations that are approximately fair. I will discuss an algorithmic framework that reconciles randomization and approximation. Specifically, I will present an algorithm for finding a randomized allocation of indivisible goods that is ex-ante fair, i.e., envy-free in expectation, and ex-post approximately fair, i.e., envy-free up to one good.

<https://arxiv.org/abs/2005.14122>

<https://arxiv.org/abs/2004.02554>

## [01408] Strong Revenue (Non-)Monotonicity of Single-parameter Auctions

**Author(s)** : Ziyun Chen (Tsinghua University)Zhiyi Huang (The University of Hong Kong)Dorsa Majdi (Sharif University of Technology)Zipeng Yan (The University of Hong Kong)

**Abstract** : Consider Myerson's optimal auction with respect to an inaccurate prior, e.g., estimated from data, which is an underestimation of the true value distribution. Can the auctioneer expect getting at least the optimal revenue w.r.t. the inaccurate prior since the true value distribution is larger? This so-called strong revenue monotonicity is known to be true for single-parameter auctions when the feasible allocations form a matroid. We find that strong revenue monotonicity fails to generalize beyond the matroid setting, and further show that auctions in the matroid setting are the only downward-closed auctions that satisfy strong revenue monotonicity. On the flip side, we recover an approximate version of strong revenue monotonicity that holds for all single-parameter auctions, even without downward-closedness. As applications, we get sample complexity upper bounds for single-parameter auctions under matroid constraints, downward-closed constraints, and general constraints. They improve the state-of-the-art upper bounds and are tight up to logarithmic factors.

## [01426] Tract housing, the core, and pendulum auctions

**Author(s)** : Andrew Mackenzie (\*Department of Microeconomics and Public Economics, Maastricht University)Yu Zhou (Graduate School of Economics, Kyoto University)

**Abstract** : We consider a model of tract housing where buyers and sellers have (i) wealth constraints, and (ii) unit demand over identical indivisible objects represented by a valuation. First, we characterize the strong core. Second, we characterize the bilateral weak core, or the weak core allocations with no side-payments. Finally, when buyer wealth constraints and valuations are private information and when transfers are discrete, we introduce two families of pendulum auctions, both of which consist of obviously strategy-proof implementations of the bilateral weak core. The buyer-optimal pendulum auctions are preferred by the buyers but are inefficient when side-payments are possible, while the efficient pendulum auctions are efficient.

## [01516] Are Simple Mechanisms Optimal when Agents are Unsophisticated?

**Author(s)** : Jiangtao Li (Singapore Management University)Piotr Dworczak (Northwestern University)

**Abstract** : We study the design of mechanisms involving agents that have limited strategic sophistication. We define a mechanism to be simple if—given the assumed level of strategic sophistication—agents can determine their optimal strategy. We examine whether it is optimal for the mechanism designer who faces strategically unsophisticated agents to offer a simple mechanism. We show that when the designer uses a mechanism that is not simple, while she loses the ability to predict play, she may nevertheless be better off no matter how agents resolve their strategic confusion.

## [01530] Representation Theorems for Path-Independent Choice Rules

**Author(s)** : Koji Yokote (The University of Tokyo)Isa E. Hafalir (University of Technology Sydney)Fuhito Kojima (The University of Tokyo)M. Bumin Yenmez (Boston College)

**Abstract** : Path independence is arguably the most important property of choice rules in market design. For example, it guarantees the existence of a desirable matching in two-sided markets. We show that a choice rule is path independent if and only if it is rationalized by a valuation function satisfying ordinal concavity. We also provide a representation result for choice functions that satisfy path independence and the law of aggregate demand using valuation functions satisfying ordinal concavity.

## [01616] Optimal Dynamic Matching

**Author(s)** : Junpei Komiyama (New York University)Akira Matsushita (The University of Tokyo)Shunya Noda (The University of Tokyo)

**Abstract** : We propose a machine-learning method to construct an approximately optimal algorithm for a general class of dynamic matching problems. We apply our method to several problems and compare an algorithm generated by our method with simplistic ones, such as a greedy algorithm, to illustrate the importance of optimizing allocations in dynamic environments.

00715 (3/3) : 2E @D505

## [01620] Multi-Unit Bilateral Trade

**Author(s)** : Bart de Keijzer (King's College London)

**Abstract** : We characterise the set of dominant strategy incentive compatible (DSIC), strongly budget balanced (SBB), and ex-post individually rational (IR) mechanisms for the multi-unit bilateral trade setting. In such a setting there is a single buyer and a single seller who holds a finite number  $k$  of identical items. The mechanism has to decide how many units of the item are transferred from the seller to the buyer and how much money is transferred from the buyer to the seller. We consider two classes of valuation functions for the buyer and seller: Valuations that are increasing in the number of units in possession, and the more specific class of valuations that are increasing and submodular.

Furthermore, we present some approximation results about the performance of certain such mechanisms, in terms of social welfare: For increasing submodular valuation functions, we show the existence of a deterministic 2-approximation mechanism and a randomised  $e/(1 - e)$  approximation mechanism, matching the best known bounds for the single-item setting.

Joint work with Matthias Gerstgrasser, Paul Goldberg, Philip Lazos, and Alexander Skopalik. Based on a paper published in the Proceedings of AAAI 2019.

## [01693] Mechanism Design Powered by Social Interactions

**Author(s)** : Dengji Zhao (ShanghaiTech University)

**Abstract** : Mechanism design has traditionally assumed that the participants are fixed and independent. However, in reality, the participants are well-connected (e.g., via their social networks) and we can utilize their connections to power the design. One interesting trend is to incentivize the existing participants to use their connections to invite new participants. This helps to form larger games in auctions, coalitional games, matching etc., which is not achievable with the traditional solutions. The challenge is that the participants are competitors and they would not invite each other by default. Solving this is well-coupled with the existing challenges. For example, in auctions, solving it may require revenue monotonicity and false-name-proofness, which were proved impossible to achieve under certain sensible conditions. In matching, this cannot get along with standard optimality and stability. Hence, we believe there is an important theoretical value to discover and the study will stimulate many interesting applications, especially under decentralized systems with blockchain.

## [01738] Optimal allocation with costly verification and distributional constraint

**Author(s)** : Yunan Li (City University of Hong Kong)

**Abstract** : A planner allocates multiple slots (e.g., a spot in college) among a finite number of agents, each of whom wants one slot and privately knows the value to the planner of assigning one slot to him. The slots are allocated based on the agents' reports. The planner can choose to inspect an agent's report at a cost. The constrained efficient mechanism for a planner facing a distributional constraint adds a constant to the values of the agents in the targeted group (a "flat subsidy") and specifies a threshold. The slots are first allocated to the agents whose (adjusted) values are above the threshold. Any remaining slots are randomly allocated among the agents whose (adjusted) values are below the threshold. For a stringent distributional constraint, the randomization favors the targeted group (a "quota").

## [05446] Strategyproof Mechanisms for Group-Fair Facility Location Problems

**Author(s)** : Minming Li (City University of Hong Kong) Houyu Zhou (City University of Hong Kong) Hau Chan (University of Nebraska-Lincoln)

**Abstract** : We study the facility location problems where agents are located on a real line and divided into groups based on criteria such as ethnicity or age. Our aim is to design mechanisms to locate a facility to approximately minimize the costs of groups of agents to the facility fairly while eliciting the agents' locations truthfully. We first explore various well-motivated group fairness cost objectives for the problems and show that many natural objectives have an unbounded approximation ratio. We then consider minimizing the maximum total group cost and minimizing the average group cost objectives. For these objectives, we show that existing classical mechanisms (e.g., median) and new group-based mechanisms provide bounded approximation ratios, where the group-based mechanisms can achieve better ratios. We also provide lower bounds for both objectives. To measure fairness between groups and within each group, we study a new notion of intergroup and intragroup fairness (IIF). We consider two IIF objectives and provide mechanisms with tight approximation ratios.

## [00718] Data-driven and physics-informed techniques in Data Assimilation

**Session Time & Room :**

00718 (1/3) : 1C (Aug.21, 13:20-15:00) @E817

00718 (2/3) : 1D (Aug.21, 15:30-17:10) @E817

00718 (3/3) : 1E (Aug.21, 17:40-19:20) @E817

**Type** : Proposal of Minisymposium

**Abstract** : In light of the great proliferation of data and increase in computational power, the importance of effectively combining observations with dynamical models for the purpose of prediction, parameter estimation, and modeling remains a fundamental challenge. Exciting recent works at the interface of machine learning, analysis of PDEs, and data assimilation have led to the development of new methods, analytic insights and unifying perspectives, as well as novel applications. This mini-symposium will bring together researchers that have made such contributions in analytical or computational capacities.

**Organizer(s)** : Jochen Broecker, Vincent Martinez, Sahani Pathiraja

**Classification** : 68T07, 65M32, 35Q62, 62F15, 76D55

**Minisymposium Program :**

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00718 (1/3) : 1C @E817 [Chair: Vincent Martinez]

## [02864] Consistency Results for some Bayesian PDE inverse problems

**Format** : Online Talk on Zoom

**Author(s)** : Nathan Glatt-Holtz (Tulane)

**Abstract** : Frequently one would like to estimate functional parameters  $u$  in a physical model defined by a partial differential equation from a collection of sparse and uncertain observations. Here a Bayesian methodology provides an attractive statistical approach for many such estimation problems, one which provides a comprehensive picture of uncertainties in the unknown. An important step in the validation of this Bayesian methodology is to establish conditions for posterior consistency. Specifically we would like to determine when  $\mu_N \rightharpoonup \delta_{u_*}$  where  $\mu_N$  is the Bayesian posterior conditioned on  $N$  observations of the solution and  $u_*$  is the true value of the unknown.

In this talk we describe some rigorous approaches that we have recently developed tailored to address consistency for PDE inverse problems involving the recovery of an infinite dimensional unknown. We describe how our approach applies to a gallery of model problems including the recovery of a divergence free velocity field from the measurement of a solute which is advecting and diffusing in the fluid medium. This is joint work with Jeff Borggaard, Christian Frederiksen and Justin Krometis.

## [05063] Data-driven and model-driven techniques in DA: applications, numerics, rigorous results

**Format :** Online Talk on Zoom

**Author(s) :** Jochen Broecker (Department of Mathematics and Statistics, University of Reading)

**Abstract :** Data Assimilation permeates all contributions in at least three ways: Firstly, novel approaches to data assimilation use machine learning and Bayesian inference to identify the current state as well as components of the system, two inextricably linked aims. Secondly, data assimilation has become an interesting application of (stochastic) PDE-theory. Thirdly, ergodic theory of infinite dimensional dynamical systems (asymptotic coupling) calls for sophisticated nudging or error feedback schemes. Finally, new venues for research will be sketched.

## [02753] Nonparametric Bayesian inference of discretely observed diffusions

**Format :** Talk at Waseda University

**Author(s) :** Jean-Charles Croix (Amazon)Masoumeh Dashti (University of Sussex)Stylianos Katsarakis (University of Sussex)Istvan Kiss (University of Sussex)Tanja Zerenner (University of Bristol)

**Abstract :** We consider the inverse problem of recovering the diffusion and drift functions of a stochastic differential equation from discrete measurements of its solution. We show the stability of the posterior measure with respect to appropriate approximations of the underlying forward model allowing for priors with unbounded support. We then look at the approximated posterior obtained by Gaussian approximation of transition densities in the case where the diffusion coefficient is small.

## [02850] A general involution framework for Metropolis-Hastings algorithms and applications to Bayesian inverse problems

**Format :** Talk at Waseda University

**Author(s) :** Cecilia Mondaini (Drexel University)Nathan Glatt-Holtz (Tulane University)

**Abstract :** We consider a general framework for Metropolis-Hastings algorithms used to sample from a given target distribution on a general state space. Our framework has at its core an involution structure, and is shown to encompass several popular algorithms as special cases, both in the finite- and infinite-dimensional settings. In particular, it includes random walk, preconditioned Crank-Nicolson (pCN), schemes based on a suitable Langevin dynamics such as the Metropolis Adjusted Langevin algorithm (MALA), and also ones based on Hamiltonian dynamics including several variants of the Hamiltonian Monte Carlo (HMC) algorithm. In addition, our framework comprises algorithms that generate multiple proposals at each iteration, which allow for greater efficiency through the use of modern parallel computing resources. Aside from encompassing existing algorithms, we also derive new schemes from this framework, including some multiproposal versions of the pCN algorithm. To illustrate effectiveness of these sampling procedures, we present applications in the context of certain Bayesian inverse problems in fluid dynamics. In particular, we consider the problem of recovering an incompressible background fluid flow from sparse and noisy measurements of the concentration of a passive solute advected by the flow. This talk is based on joint works with N. Glatt-Holtz (Tulane U), A. Holbrook (UCLA), and J. Krometis (Virginia Tech).

00718 (2/3) : 1D @E817 [Chair: Jochen Broecker]

## [02843] Insights from Nonlinear Continuous Data Assimilation for Turbulent Flows

**Format :** Talk at Waseda University

**Author(s) :** Elizabeth Carlson (University of Victoria)Adam Larios (University of Nebraska - Lincoln)Edriss S Titi (University of Cambridge)

**Abstract :** One of the challenges of the accurate simulation of turbulent flows is that initial data is often incomplete. Data assimilation circumvents this issue by continually incorporating the observed data into the model. An emerging approach to data assimilation known as the Azouani-Olson-Titi (AOT) algorithm introduced a feedback control term to the 2D incompressible Navier-Stokes equations (NSE) in order to incorporate sparse measurements. The solution to the AOT algorithm applied to the 2D NSE was proven to converge exponentially to the true solution of the 2D NSE with respect to the given initial data. In this talk, we will focus on the insights of a nonlinear version of the AOT algorithm and distinguish the clear connections to the physics of the existing systems.

## [02852] Linear response for nonlinear dissipative SPDEs

**Format :** Talk at Waseda University

**Author(s) :** Giulia Carigi (University of L'Aquila)Jochen Bröcker (University of Reading)Tobias Kuna (University of L'Aquila)

**Abstract :** A framework suitable to establish response theory for a class of nonlinear stochastic partial differential equations is provided, exploiting coupling methods. The results are applied to the 2D stochastic Navier-Stokes equation and the stochastic two-layer quasi-geostrophic model. In particular, studying the response to perturbations in the forcings for models in geophysical fluid dynamics gives a mathematical insight into whether statistical properties derived under current conditions will be valid under different forcing scenarios.

## [05078] Data assimilation of the 2D rotating NSE

**Format :** Talk at Waseda University

**Author(s) :** Aseel Farhat (Florida State University)

**Abstract :** With sufficiently fast rotation, the solution of the 2D rotating NSE on the  $\beta$  plane approaches a nearly zonal state. Additionally, the number of degrees of freedom of the system decrease with faster rotation. We validate this analytically and numerically in the context of a continuous data assimilation algorithm based on nudging.

## [02847] Using machine learning in geophysical data assimilation (some of the issues and some ideas)

**Format :** Online Talk on Zoom

**Author(s) :** Alberto Carrassi (Dept of Physics, University of Bologna)

**Abstract :** We show how ML can be included in the prediction and DA workflow in different ways. First, in “non-intrusive” ML, we show how supervised ML estimates the local Lyapunov exponents. ML is then combined with DA in an integrated fashion to learn a surrogate model from noisy and sparse data, and a parametrization of a physical’s model unresolved scales. DA is pivotal to extract information from the sparse, noisy, data that ML cannot handle alone.

00718 (3/3) : 1E @E817 [Chair: Sahani Pathiraja]

## [02853] Almost Sure Error Bounds for Data Assimilation in Dissipative Systems with Unbounded Observation Noise

**Format :** Online Talk on Zoom

**Author(s) :** Tobias Kuna (Universita dell'Aquila)Jochen Broecker (University of Reading)Lea Oljaca (sustainable investment research)

**Abstract :** Data assimilation is widely used technique, in particular, in the geophysical community. It aims at inferring information of a model by combining incomplete and noisy observations with imperfect models even for very large models and often on the fly in real time. This methods have been extensively studied for a plethora of models, assimilation methods and error terms. In this talk, I will concentrate on how one can treat unbounded noise in the observations not only in expectation, but actually I will present a technique to obtain an a.s. bound. More specifically, we prove that the error is bounded by a finite and stationary processes. We use the simple replacement data assimilation scheme by Hayden, Olson and Titi, see [1] with observations discrete in time, including but not limited to 2D Navier-Stokes equation. The method should extend to more general algorithms like described in [2], as its estimates are based on absorbing and squeezing properties generalizing [3]. The content of the talk was published in [4].

- [1] K. Hayden, E. Olson, and E. S. Titi, Discrete data assimilation in the Lorenz and 2D Navier-Stokes equations, Phys. D, 240 (2011), pp. 1416–1425
- [2] D. Sanz-Alonso and A. M. Stuart, Long-time asymptotics of the filtering distribution for partially observed chaotic dynamical systems, SIAM/ASA J. Uncertain. Quantif., 3 (2015), pp. 1200–1220,
- [3] C. E. A. Brett, K. F. Lam, K. J. H. Law, D. S. McCormick, M. R. Scott, and A. M. Stuart, Accuracy and stability of filters for dissipative PDEs, Phys. D, 245 (2013), pp. 34–45,
- [4] L. Oljača, J. Bröcker and T. Kuna, Almost sure error bounds for data assimilation in dissipative systems with unbounded observation noise, IAM J. Appl. Dyn. Syst., 17(4) (2018) pp. 2882–2914.

## [04934] Challenges in high dimensional nonlinear filtering

**Format :** Talk at Waseda University

**Author(s) :** Jana de Wiljes (Uni Potsdam)

**Abstract :** The seamless integration of large data sets into computational models is one of the central challenges for the mathematical sciences of the 21st century.

Despite the fact that the underlying assumptions do not hold for many applications, Gaussian approximative filters are considered state of the art as they have been successfully implemented for highly nonlinear settings with large

dimensional state spaces. Moreover several recent studies have been devoted to showing accuracy of such filters in terms of tracking ability for nonlinear evolution models and we will present one of these results given in the form of distinct bounds for certain filter variants.

While the robustness of such Gaussian approximative filters is undeniable there has been considerable aspiration to design filters that can achieve even higher levels of accuracy while maintaining an appropriate level of robustness and stability.

Here we will discuss a family of such filters that do not require a parametrization of the posterior distribution and can be combined with traditional Gaussian filters via a likelihood split.

## [02745] Particle Filters for Data Assimilation

**Format :** Online Talk on Zoom

**Author(s) :** Dan Crisan (Imperial College London )

**Abstract :** I will present the latest developments of on-going work on the application of particle filters to develop high dimensional data assimilation methodologies.

## [04884] A novel regularity criterion for the 3D Navier-Stokes equations based on finitely many observations.

**Format :** Online Talk on Zoom

**Author(s) :** Animikh Biswas (University of Maryland Baltimore County)Abhishek Balakrishna (University of Maryland Baltimore County)

**Abstract :** We present a novel regularity criterion for the 3D Navier-Stokes equations (NSE) based on finitely many modal, nodal or volume element observations of the velocity field. The proof is based on a data assimilation algorithm utilizing a Newtonian relaxation scheme (nudging) motivated by feedback-control. The observations, which may be either modal, nodal or volume elements, are obtained from a weak solution of the 3D NSE and are collected almost everywhere in time over a finite grid. The regularity criterion we propose follows from our data assimilation algorithm and is hence intimately connected to the notion of determining functionals (modes, nodes and volumeelements). To the best of our knowledge, all existing regularity criteria require knowing the solutionof the 3D NSE almost everywhere in space. Our regularity criterion is fundamentally different fromany preexisting regularity criterion as it is based on finitely many observations (modes, nodes andvolume elements). We further prove that the regularity criterion we propose is both a necessaryand sufficient condition for regularity. Thus our result can be viewed as a natural generalizationof the notion of determining modes, nodes and volume elements as well as the asymptotic trackingproperty of the nudging algorithm for the 2D NSE to the 3D setting.

## [00719] Recent Advances in Numerical PDE and Scientific Machine Learning

**Session Time & Room :**

00719 (1/2) : 3E (Aug.23, 17:40-19:20) @E702

00719 (2/2) : 4C (Aug.24, 13:20-15:00) @E702

**Type :** Proposal of Minisymposium

**Abstract :** Artificial intelligence is constantly evolving and researchers are utilizing deep neural networks in increasingly complex problem sets. To address the difficulties posed by these new setups, deep learning research is exploring new modeling tools, including differential equations, to improve the predictive capabilities of neural networks. These technologies have demonstrated potential in speeding up scientific simulations and achieved state-of-the-art performance in various fields. This minisymposium will focus on recent developments in the intersection of scientific computing and deep learning, highlighting their impact and application across multiple disciplines.

**Organizer(s) :** Minseok Choi, Youngjoon Hong

**Classification :** 65M22, 68T07, 65K05, 68T09, Scientific Machine Learning

**Minisymposium Program :**

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00719 (1/2) : 3E @E702 [Chair: Youngjoon Hong]

## [04237] Level set learning for nonlinear dimensionality reduction in function approximation

**Format :** Talk at Waseda University

**Author(s) :** Zhu Wang (University of South Carolina)

**Abstract :** Approximating high-dimensional functions is challenging due to the curse of dimensionality. Inspired by the Nonlinear Level set Learning method that uses the reversible residual network, we developed a new method, Dimension Reduction via Learning Level Sets, for function approximations. It contains two major components: one is the pseudo-reversible neural network module that effectively transforms high-dimensional input variables to low-dimensional active variables, and the other is the synthesized regression module for approximating function values based on the transformed data in the low-dimensional space. Numerical experiments will be presented to demonstrate the proposed method.

## [03271] Semi-analytic PINN methods for boundary layer problems on rectangular domains

**Format :** Talk at Waseda University

**Author(s) :** Chang-Yeol Jung (UNIST)Gung-Min Gie (University of Louisville)Youngjoon Hong (Sungkyunkwan University)Tselmuun Munkhjin (UNIST)

**Abstract :** Singularly perturbed boundary value problems exhibit sharp boundary layers in their solutions, making their numerical approximation challenging due to the stiffness of these layers, resulting in significant computational errors. Traditional numerical methods require extensive mesh refinements near the boundary to obtain accurate solutions, which can be costly in terms of computation.

To address these challenges, we have employed physics-informed neural networks (PINNs) to solve singularly perturbed problems. However, PINNs can struggle with rapidly varying singularly perturbed solutions over a small domain region, resulting in insufficient resolution that can lead to inaccurate results. To overcome this limitation, we consider the semi-analytic methods which enrich the PINNs with so-called corrector functions. Our numerical experiments demonstrate significant improvements in accuracy and stability.

## [04847] Solving Wave Equations with Fourier Neural Operator

**Format :** Talk at Waseda University

**Author(s) :** Bian Li (Lehigh University)Hanchen Wang (Los Alamos National Lab)Shihang Feng (Los Alamos National Lab)Xiu Yang (Lehigh University)Youzuo Lin (Los Alamos National Lab)

**Abstract :** In the study of subsurface seismic imaging, solving the acoustic wave equation is a pivotal component in existing models. Inspired by the idea of operator learning, this work leverages the Fourier neural operator (FNO) to effectively learn the frequency domain seismic wavefields under the context of variable velocity models. We also propose a new framework paralleled Fourier neural operator (PFNO) for efficiently training the FNO-based solver given multiple source locations and frequencies.

## [04931] Physics-informed variational inference for stochastic differential equations

**Format :** Talk at Waseda University

**Author(s) :** Hyomin Shin (POSTECH)Minseok Choi (POSTECH)

**Abstract :** In this talk, we propose a physics-informed learning based on variational autoencoder (VAE) to solve data-driven stochastic differential equations. We adopt VAE to extract the random state of the governing equation, and train the model by maximizing the evidence lower bound that incorporates the given physical laws. We present numerical examples to demonstrate the effectiveness of the proposed method.

00719 (2/2) : 4C @E702 [Chair: Minseok Choi]

## [03076] Deep neural operator for learning transient response of composites subject to dynamic loading

**Format :** Online Talk on Zoom

**Author(s) :** Zhen Li (Clemson University)Minglei Lu (Clemson University)Ali Mohammadi (Clemson University)Zhaoxu Meng (Clemson University)Gang Li (Clemson University)

**Abstract :** Deep neural operator (DNO) is used learn the transient response of composites as surrogate of physics-based finite element analysis (FEA). We consider a 3D composites beam formed by two metals with different Young's modulus subject to dynamic loads. DNO is trained using sequence-to-sequence learning with incremental learning methods based on 5000 FEA data, leading to a 100X speedup. Results show that DNO can predict the transient mechanical response of composites at an accuracy of 97%.

## [05598] Analysis of the derivative-free method for solving PDEs using neural networks

**Format :** Talk at Waseda University

**Author(s) :** Jihun Han (Dartmouth College)Yoonsang Lee (Dartmouth College)

**Abstract :** The derivative-free loss method (DFLM) uses a stochastic (Feynman-Kac) formulation to solve a certain class of PDEs using neural networks. The method avoids the derivative calculation from neural networks, using statistical information of local walkers to represent the solution. This work analyzes the effect of the time step and the number of walkers in DFLM. The analysis shows a lower bound for the time step to guarantee a certain accuracy, which contrasts the standard numerical methods with an upper bound. We also show a linear dependence of the walker in the accuracy.

## [03762] Convergence analysis of unsupervised Legendre-Galerkin neural networks for linear second-order elliptic PDEs

**Format :** Talk at Waseda University

**Author(s) :** Seungchan Ko (Inha University)Seok-Bae Yun (Sungkyunkwan University)Youngjoon Hong (Sungkyunkwan University)

**Abstract :** In this talk, I will discuss the convergence analysis of unsupervised Legendre-Galerkin neural networks (ULGNet), a deep-learning-based numerical method for solving partial differential equations (PDEs). Unlike existing deep learning-based numerical methods for PDEs, the ULGNet expresses the solution as a spectral expansion with respect to the Legendre basis and predicts the coefficients with deep neural networks by solving a variational residual minimization problem. Using the fact that the corresponding loss function is equivalent to the residual induced by the linear algebraic system depending on the choice of basis functions, we prove that the minimizer of the discrete loss function converges to the weak solution of the PDEs. Numerical evidence will also be provided to support the theoretical result. Key technical tools include the variant of the universal approximation theorem for bounded neural networks, the analysis of the stiffness and mass matrices, and the uniform law of large numbers in terms of the Rademacher complexity.

## [04540] Bi-orthogonal fPINN: A physics-informed neural network method for solving time-dependent stochastic fractional PDEs

**Format :** Talk at Waseda University

**Author(s) :** Lei Ma (Shanghai normal university)

**Abstract :** Mathematical models considering nonlocal interactions with uncertainty quantification can be formulated as stochastic fractional partial differential equations (SFPDEs). There are many challenges in solving SFPDEs numerically, especially for long-time integration. Here, we combine the bi-orthogonal (BO) method for representing stochastic processes with physics-informed neural networks (PINNs) for solving partial differential equations to formulate the bi-orthogonal PINN method (BO-fPINN) for solving time-dependent SFPDEs. We demonstrate the effectiveness of the BO-fPINN method for different benchmark problem.

# [00721] Data-driven and Model Reduction methods for Subsurface Applications

**Session Time & Room :**

00721 (1/2) : 2E (Aug.22, 17:40-19:20) @E703

00721 (2/2) : 3C (Aug.23, 13:20-15:00) @E703

**Type :** Proposal of Minisymposium

**Abstract :** There are recently a lot of exciting new computational approaches with the aim of solving practical and challenging subsurface applications such as multiphase flow in a fractured reservoir as well as geothermal modeling with heat conduction. The aim of this mini-symposium is to review recent progress in data-driven and model-reduction methods like multiscale methods, numerical upscaling techniques, and learning-based algorithms for related applications and motivate new research directions in solving challenging problems from the field of computational geosciences.

**Organizer(s) :** Siu Wun Cheung, Wing Tat Leung, Sai-Mang Pun

**Classification :** 65M60, 65N30, 76S05, 86-08

**Minisymposium Program :**

## [04298] Deep Learning Methods for PDEs and Reduced Order Models

**Format :** Talk at Waseda University

**Author(s) :** Min Wang (University of Houston)

**Abstract :** In this talk, we will discuss the use of neural networks to solve high-dimensional partial differential equations (PDEs) without being affected by the curse of dimensionality. We will explore three key questions: (1) How to formulate PDE problems as optimization problems for deep learning techniques, (2) The accuracy of neural network approximations, and (3) Systematic training for global minimum convergence. In specific, We will present various optimization formulations for the high-dimensional quadratic porous medium equation, analyze generalization and approximation errors for Ritz methods, and propose an adaptive optimization strategy for training residual neural networks. Numerical results will be provided to demonstrate the effectiveness of the proposed methods.

## [03429] Nonlocal multicontinua with representative volume elements

**Format :** Talk at Waseda University

**Author(s) :** Wing Tat Leung (City University of Hong Kong)

**Abstract :** In this talk, we present a general derivation of multicontinuum equations and discuss cell problems. We present constraint cell problem formulations in a representative volume element and oversampling techniques that allow reducing boundary effects. We discuss different choices of constraints for cell problems. We present numerical results that show how oversampling reduces boundary effects. Finally, we discuss the relation of the proposed methods to our previously developed methods, Nonlocal Multicontinuum Approaches.

## [05249] Physics-informed neural networks for learning the homogenized coefficients of multiscale elliptic equations

**Format :** Online Talk on Zoom

**Author(s) :** Jun Sur Richard Park (KAIST)Xueyu Zhu (Department of Mathematics, University of Iowa)

**Abstract :** Multiscale elliptic equations with scale separation are often approximated by the corresponding homogenized equations with slowly varying homogenized coefficients (the G-limit). The traditional homogenization techniques typically rely on the periodicity of the multiscale coefficients, thus finding the G-limits often requires sophisticated techniques in more general settings even when the multiscale coefficient is known, if possible. Our approach adopts physics-informed neural networks (PINNs) algorithm to estimate the G-limits from the multiscale solution data by leveraging a priori knowledge of the underlying homogenized equations. Unlike the existing approaches, our approach does not rely on the periodicity assumption or the known multiscale coefficient during the learning stage. We demonstrate that the proposed approach can deliver reasonable and accurate approximations to the G-limits as well as homogenized solutions through several benchmark problems.

00721 (2/2) : 3C @E703 [Chair: Wing Tat Leung]

## [02709] Optimality of statistical criterion in hyper-reduction

**Format :** Talk at Waseda University

**Author(s) :** Siu Wun Cheung (Lawrence Livermore National Laboratory)

**Abstract :** While projection-based reduced order models can reduce the dimension of solutions, there may still be nonlinear terms which scale with the full order dimension. Hyper-reduction techniques are sampling-based methods that further reduce computational complexity of nonlinear terms. In this talk, we will view the state-of-the-art Discrete Empirical Interpolation Method from the perspective of optimal design, and introduce a new hyper-reduction method based on optimality of another statistical criterion.

## [04174] Least-squares Method for Recovering Multiple Medium Parameters

**Format :** Talk at Waseda University

**Author(s) :** Ying Liang (Purdue University)

**Abstract :** We present a two-stage least-squares method for inverse medium problems of reconstructing multiple unknown coefficients simultaneously from noisy data. A direct sampling method is applied to detect the location of the inhomogeneity in the first stage, while a total least-squares method with a mixed regularization is used to recover the medium profile in the second stage. The total least-squares method is designed to minimize the residual of the model equation and the data fitting, along with an appropriate regularization, in an attempt to significantly improve the accuracy of the approximation obtained from the first stage. We shall also present an analysis on the well-posedness and convergence of this algorithm. Numerical experiments are carried out to verify the accuracies and robustness of this novel two-stage least-squares algorithm, with high tolerance of noise in the data.

## [03801] Adaptive partially explicit splitting scheme for multiscale flow problems

**Format :** Online Talk on Zoom

**Author(s) :** Yating Wang (Xi'an Jiaotong University)Wing Tat Leung (City University of Hong Kong)

**Abstract :** In this talk, we will introduce an adaptive framework for a partially explicit splitting scheme of flow problems in high-contrast multiscale media. Due to the heavy computational burden is for the multiscale coefficient with high-contrast, in this work, we utilize a stable multirate temporal splitting scheme, and construct multiscale subspaces to handle the fast flow and slow flow parts separately. The construction of multiscale spaces ensures that the time-step size is independent of the contrast. We then derive both temporal and spatial error estimators to identify local regions where enrichments are needed for two components of the solutions. An adaptive algorithm is then proposed to achieve higher computational efficiency with the desired accuracy.

## [00727] Recent Advances in Fast Iterative Methods for PDE Problems

**Session Time & Room :**

00727 (1/3) : 4C (Aug.24, 13:20-15:00) @E701

00727 (2/3) : 4D (Aug.24, 15:30-17:10) @E701

00727 (3/3) : 4E (Aug.24, 17:40-19:20) @E701

**Type :** Proposal of Minisymposium

**Abstract :** Solving vast sparse or structured linear systems is one of the major tasks when solving partial differential equation (PDE) problems in many applications in science and engineering. Iterative solvers such as Krylov subspace methods and the multigrid methods, with effective preconditioners, are often used for solving these linear systems efficiently. This minisymposium brings various researchers and experts in these areas together to present the latest development of iterative methods, preconditioners, and linear algebra software.

**Organizer(s) :** Sean Hon, Xuelei Lin

**Classification :** 65M06, 65M22, 65F08, 65F10

**Minisymposium Program :**

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00727 (1/3) : 4C @E701 [Chair: Sean Hon]

## [02883] Multigrid Methods for Saddle-Point Matrices with Structured Blocks

**Format :** Talk at Waseda University

**Author(s) :** Isabella Furci (University of Genoa)Matthias Bolten (University of Wuppertal)Marco Donatelli (University of Insubria)Paola Ferrari (University of Wuppertal)

**Abstract :** We consider efficient multigrid methods for large linear systems with particular saddle-point structures. Often, powerful smoothers are used to take into account the special coupling. Alternatively, Notay recently proposed an algebraic approach that analyzes properly preconditioned saddle-point problems.

We provide theoretical tools to analyze the latter procedure when applied to saddle-point systems whith (multilevel) block-Toeplitz blocks. As a test problem, we consider the linear system stemming from the Finite Element approximation of the Stokes equation.

## [05299] New Linear Solvers Features and Improvements in Trilinos

**Format :** Online Talk on Zoom

**Author(s) :** Jennifer Ann Loe (Sandia National Laboratories)Ichitaro Yamazaki (SNL)Sivasankaran Rajamanickam (Sandia National Laboratories)Heidi Thornquist (Sandia National Laboratories)Christian Glusa (Sandia National Laboratories)

**Abstract :** Trilinos is a large open-source mathematical software library which includes algorithms for discretization, optimization, preconditioners, non-linear solvers, and linear solvers. Its Tpetra linear algebra backend allows it to run effectively on highly parallel computers and various GPU accelerators. In this talk, we discuss recent improvements and additions to the Trilinos linear solver capabilities. One addition allows mixed precision solver and preconditioner combinations. Another recent improvement provides an abstract interface for small dense matrices in the linear solvers, eliminating extra data movement for GPU-based computers. We will demonstrate potential performance gains with use of the new linear solvers features.

## [04769] A rational preconditioner for multi-dimensional Riesz fractional diffusion equations

**Format :** Online Talk on Zoom

**Author(s) :** Mariarosa Mazza (University of Insubria)Lidia Aceto (University of Eastern Piedmont)

**Abstract :** Starting from a rational approximation of the Riesz operator expressed as the integral of the standard heat diffusion semigroup, we propose a rational preconditioner for solving linear systems arising from the finite difference/element discretization of multi-dimensional Riesz fractional diffusion equations. We show that, despite the lack of clustering just as for the Laplacian, for fractional orders close to 1 our preconditioner provides better results than the Laplacian itself, while sharing the same computational complexity.

## [02906] Some step-size independent theoretical bounds for preconditioning techniques of discrete PDEs

**Format :** Talk at Waseda University

**Author(s) :** Xuelei Lin (Harbin Institute of Technology Shenzhen)

**Abstract :** It is well-known that the condition number of coefficient matrices arising from discretization of differential equations increases as the grid gets refined, because of which iterative solvers converge slowly for the linear systems when the grid is dense. In this talk, preconditioning techniques for discretization of some differential equations are introduced, with which some Krylov subspace solvers for the preconditioned systems are proven to have a linear convergence rate independent of the stepsizes. Numerical results are also reported.

00727 (2/3) : 4D @E701 [Chair: Xuelei Lin]

## [04605] A single-sided all-at-once preconditioning for linear system from a non-local evolutionary equation with weakly singular kernels

**Format :** Talk at Waseda University

**Author(s) :** Xuelei Lin (Harbin Institute of Technology Shenzhen)Jiamei Dong (Hong Kong Baptist University)Sean Hon (Hong Kong Baptist University)

**Abstract :** We propose a preconditioning technique for the multilevel Toeplitz all-at-once linear system arising from a time-space fractional diffusion equation. The preconditioning technique is based on replacing the spatial discretization matrix with  $\alpha$ -matrix, due to which the preconditioner can be fast inverted. Theoretically, we show that the condition number of the intermediate two-sided preconditioned matrix is bounded by 3. And the norm of our preconditioner residual is bounded by the residual of intermediate preconditioner .

## [04933] Fast algorithms for space fractional Cahn-Hilliard equations

**Format :** Online Talk on Zoom

**Author(s) :** Xin Huang (Huazhong University of Science and Technology)

**Abstract :** In this talk, the space fractional Cahn-Hilliard (CH) equation is considered. Combining the scale auxiliary variable (SAV) technique with the leapfrog scheme, an unconditional energy-stable, non-couple and linearly implicit numerical scheme is derived. The fully-discrete scheme gives rise to an ill-conditioned system. The Krylov subspace method combining with the preconditioning technique is adopted to solve the resulting system. Numerical results are given to show the efficiency of the proposed method.

## [05262] A parallel preconditioner for the all-at-once linear system from evolutionary PDEs with Crank-Nicolson discretization in time

**Format :** Online Talk on Zoom

**Author(s) :** Xian-Ming Gu (Southwestern University of Finance and Economics)Yong-Liang Zhao (Sichuan Normal University)

**Abstract :** The Crank-Nicolson (CN) method is a fashionable time integrator for evolutionary partial differential equations (PDEs) arisen in many areas of applied mathematics, however since the solution at any time depends on the solution at previous time steps, thus the CN method will be inherently difficult to parallelize. In this talk, we consider a parallel approach for the solution of evolutionary PDEs with the CN scheme. Using an all-at-once approach, we can solve for all time steps simultaneously using a parallelizable over time preconditioner within a standard iterative method. Due to the diagonalization of the proposed preconditioner, we can minutely prove that most eigenvalues of preconditioned matrices are equal to 1 and the others  $z \in \mathbb{C}$  have the model with  $1/(1 + \alpha) < |z| < 1/(1 - \alpha)$ , where  $0 < \alpha < 1$  is a free parameter. Meanwhile, the efficient and parallel implementation of this proposed preconditioner is described in details. Finally, we will verify our theoretical findings via numerical experiments.

## [05468] A preconditioned MINRES method for optimal control of wave equations

**Format :** Talk at Waseda University

**Author(s) :** Sean Hon (Hong Kong Baptist University)

**Abstract :** In this work, we propose a novel preconditioned Krylov subspace method for solving an optimal control problem of wave equations, after explicitly identifying the asymptotic spectral distribution of the involved sequence of linear coefficient matrices from the optimal control problem. Namely, we first show that the all-at-once system stemming from the wave control problem is associated to a structured coefficient matrix-sequence possessing an eigenvalue distribution. Then, based on such a spectral distribution of which the symbol is explicitly identified, we develop an ideal preconditioner and two parallel-in-time preconditioners for the saddle point system composed of two block Toeplitz matrices. For the ideal preconditioner, we show that the eigenvalues of the preconditioned matrix-sequence all belong to the set  $(-\frac{3}{2}, -\frac{1}{2}) \cup (\frac{1}{2}, \frac{3}{2})$  well separated from zero, leading to mesh-independent convergence when the minimal residual method is employed. The proposed parallel-in-time preconditioners can be implemented efficiently using fast Fourier transforms or discrete sine transforms, and their effectiveness is theoretically shown in the sense that the eigenvalues of the preconditioned matrix-sequences are clustered around  $\pm 1$ , which leads to rapid convergence. When these parallel-in-time preconditioners are not fastly diagonalizable, we further propose modified versions which can be efficiently inverted. Several numerical examples are reported to verify our derived localization and spectral distribution result and to support the effectiveness of our proposed preconditioners.

00727 (3/3) : 4E @E701

## [03484] A block $\alpha$ -circulant based preconditioned MINRES method for evolutionary PDEs

**Author(s) :** Sean Hon (Hong Kong Baptist University)

**Abstract :** In this work, we propose a novel parallel-in-time preconditioner for an all-at-once system arising from the numerical solution of evolutionary partial differential equations (PDEs). Namely, considering the wave equation as a model problem, our main result concerns a block  $\alpha$ -circulant matrix based preconditioner that can be fast diagonalized via fast Fourier transforms, whose effectiveness is theoretically supported for the modified block Toeplitz system arising from discretizing the concerned wave equation. Namely, after first transforming the original all-at-once linear system into a symmetric one, we develop the desired preconditioner based on the spectral information of the modified matrix. Then, we show that the eigenvalues of the preconditioned matrix are clustered around 1 without any extreme outlier far away from the clusters. In other words, mesh-independent convergence is theoretically guaranteed when the minimal residual method is employed. Moreover, our proposed solver is further generalized to a full block triangular Toeplitz system which arises when a high order discretization scheme is used. Numerical experiments are given to support the effectiveness of our preconditioner, showing that the expected optimal convergence can be achieved.

This is joint work with Xuelei Lin (Harbin Institute of Technology).

# [00731] Optimal control: methods and applications

**Session Time & Room :**

00731 (1/2) : 5C (Aug.25, 13:20-15:00) @F401

00731 (2/2) : 5D (Aug.25, 15:30-17:10) @F401

**Type :** Proposal of Minisymposium

**Abstract :** This two part mini-symposium addresses theoretical aspects of optimisation of systems governed by ODEs and applications. Optimal control and the associated analysis indeed provides a framework general enough to cover the Riemannian case, and gradient flows on such manifolds, as well as the Finslerian one - in particular Zermelo type problems. It is also instrumental to deal with more singular situations involving for instance Fuller and turnpike phenomena. Two privileged domains of applications are considered: space mechanics, in connection with dynamical system analysis for mission design, and biology with a focus on micro-swimmers and bacterial growth.

**Organizer(s) :** Jean-Baptiste Caillau, Lamberto dell'Elce, Clément Moreau

**Classification :** 49K15, 70Q05, 37N25

**Minisymposium Program :**

00731 (1/2) : 5C @F401 [Chair: Clément Moreau]

## [04845] A variational approach for modelling and optimal control of electrodynamic tether motion

**Format :** Talk at Waseda University

**Author(s) :** Yana Valentinova Lishkova (University of Oxford) Mai Bando (Kyushu University) Sina Ober-Blöbaum (Paderborn University)

**Abstract :** We present a novel variational model for 6DOF spacecraft dynamics equipped with an electrodynamic tether in circular restricted three-body environment and use it to perform an optimal orbit transfer with simultaneous orbit and attitude control. We discuss the advantages of the suggested variational approach and develop an alternative multirate formulation of the model and OCP, investigating the extent to which such reformulations can reduce the computational cost of simulating and optimally controlling spacecraft in CR3BP.

## [04761] The Role of Stable Manifolds in Optimal Control under Stochastic Noise

**Format :** Talk at Waseda University

**Author(s) :** Mai Bando (Kyushu University) Shohei Morimitsu (Kyushu University) Takuro Nishimura (Kyushu University) Shinji Hokamoto (Kyushu University)

**Abstract :** This study investigates the optimal control around a hyperbolic fixed point under stochastic noise. For a deterministic system without noise, it is known that the stable manifold of a hyperbolic fixed point is the solution to the minimum-energy problem with infinite horizon. We analyze the structure of the optimal control under a stochastic noise based on path integral approach and investigate the role of the stable manifold of the hyperbolic fixed point.

## [04228] Second-order averaging of time-optimal low-thrust orbital transfers

**Format :** Talk at Waseda University

**Author(s) :** Lamberto Dell'Elce (Inria & Université Côte d'Azur)

**Abstract :** This work offers a numerical methodology to solve low-thrust orbital transfer problems. After detailing necessary conditions for optimality stemming from the Pontryagin maximum principle, a numerical methodology based on the averaging of the extremal flow of the optimal control hamiltonian is proposed. First, a one-parameter family of averaged solutions is obtained. Second, perturbations of these solutions associated to both short-periodic variations and second-order terms are computed. Finally, the magnitude of the thrust-to-mass ratio is identified by reconstructing a first-order approximation of the fast variables from the averaged solution.

## [03208] Optimization on manifolds by Riemannian gradient methods

**Format :** Talk at Waseda University

**Author(s) :** Hiroyuki Sato (Kyoto University)

**Abstract :** In this talk, we will discuss optimization on Riemannian manifolds. After introducing examples of manifold optimization problems, some recent results by the speaker will be presented. In particular, the Riemannian conjugate gradient method is a simple first-order method, which does not use the Hessian but only the gradient of the objective function, and it shows much faster convergence performance than the Riemannian steepest descent method. Reference: H. Sato, Riemannian Optimization and Its Applications, Springer, 2021.

00731 (2/2) : 5D @F401 [Chair: Lamberto Dell'Elce]

## [04787] Curvature related properties of Finsler manifolds and applications

**Format :** Talk at Waseda University

**Author(s) :** Sorin Sabau (Tokai University)

**Abstract :** Finsler manifolds are important generalizations of Euclidean and Riemannian ones with applications in different domains of mathematics, physics and engineering. In the present talk we are going to present some recent results concerning Finsler connections, curvature and relation with statistical models in the real world. We suggest possible development of information geometry on Finsler manifolds that would allow a wide range of applications.

## [03504] Optimal microswimmer control and a microfluidic control example

**Format :** Talk at Waseda University

**Author(s) :** Clement Moreau (RIMS, Kyoto University)

**Abstract :** Microscale swimmers are becoming increasingly prevalent. A natural question that arises from such swimmers, particularly those synthetic swimmers with targeted applications, is that of guidance and control.

The purpose of this presentation is to give an overview of the results of optimal control theory in the study of micro-

swimming organisms and devices. As an illustrative example, I will present time-optimal trajectories for a model of microfluidic control representing a swimmer guided through the external flow generated by a neighboring wall.

## [04894] Control Problems inspired by Biological Phenomena

**Format :** Talk at Waseda University

**Author(s) :** Tetsuya J. Kobayashi (Institute of Industrial Science, UTokyo) Takehiro Tottori (The University of Tokyo) Shuhei A Horiguchi (The University of Tokyo)

**Abstract :** In order to understand the design principles of biological systems, which sometimes demonstrate more efficient and sophisticated behaviors than engineering systems, the notion of control is indispensable. However, the control theories developed in the engineering domain under their standard assumptions can not necessarily be appropriately applied to biological phenomena, resulting in limited applicability to biological systems. In this presentation, we will discuss several extended control theories inspired by biological phenomena and their potential applications.

## [04045] Control in biology: topics in bacterial growth

**Format :** Talk at Waseda University

**Author(s) :** Jean-Baptiste Caillau (Université Côte d'Azur, CNRS, Inria, LJAD)

**Abstract :** We consider bacteria whose internal dynamics is modelled by the so-called self-replicator equations. This low dimensional ODE system accounts for the behaviour of the cell. The control mimics the allocation process of the cell that decides to use substrate either for gene expression or for its metabolism. Another control can be added to model an external action on a bio-engineered cell; thanks to optogenetics, one can for instance use light to trigger the production by the cell of a metabolite of interest. Several criteria are of interest here, particularly growth maximisation, or metabolite production. Pontryagin maximum principle allows to analyse these problems, revealing two characteristic features of these optimal control problems: Fuller phenomenon and turnpike behaviour. Some symbolic-numeric results are given to illustrate these.

Joint work with colleagues from Biocore, McTAO and MICROCOsm Inria teams. Support from the ANR is acknowledged (Maximic project).

## [00733] Compressible fluid dynamics and related PDE topics

**Session Time & Room :**

00733 (1/4) : 3C (Aug.23, 13:20-15:00) @G606

00733 (2/4) : 3D (Aug.23, 15:30-17:10) @G606

00733 (3/4) : 3E (Aug.23, 17:40-19:20) @G606

00733 (4/4) : 4C (Aug.24, 13:20-15:00) @G606

**Type :** Proposal of Minisymposium

**Abstract :** This mini-symposium is aimed to bring together the leading experts as well as promising young researchers to present their recent results in compressible fluid dynamics and related PDE topics. Key topics focus on the most challenging open problems in the compressible fluid dynamics such as existence of solutions, asymptotic stability of wave pattern and singular limits, etc. It also provides a premier interdisciplinary forum for senior and junior researchers to exchange their experiences in the study of partial differential equations coming from compressible fluid dynamics.

**Organizer(s) :** Feimin Huang, Song Jiang, Takayuki Kobayashi, Yong Wang

**Classification :** 35L65, 35Q35, 35Q85

**Minisymposium Program :**

00733 (1/4) : 3C @G606 [Chair: Feimin Huang]

## [01289] Time-asymptotic stability of Riemann solutions to the compressible Navier-Stokes equations

**Format :** Talk at Waseda University

**Author(s) :** Yi Wang (AMSS, Chinese Academy of Sciences)

**Abstract :** The talk is concerned with our recent developments on the time-asymptotic stability of generic Riemann solutions to the one-dimensional compressible Navier-Stokes equations including both isentropic and full cases.

## [01339] Stability analysis of Prandtl expansions for two dimensional MHD equations in Sobolev spaces

**Format :** Talk at Waseda University

**Author(s) :** Feng Xie (Shanghai Jiao Tong University)

**Abstract :** In this talk, I will review briefly the classical Prandtl boundary layer expansions method to analyze the structure of viscous flow under the high Reynolds number. And then I will discuss the vanishing viscosity limit of solution to initial boundary value problem for both incompressible and compressible magneto-hydrodynamics (MHD) equations in Sobolev spaces, where the velocity is always imposed the no-slip boundary condition. The effects of the normal component of magnetic field, tangential component of magnetic field, magnetic diffusion and the change of density on the mathematical analysis for stability of MHD boundary layer and vanishing viscosity limit of solution to MHD equations will be addressed.

## [01378] Global Strong and Weak Solutions to Compressible MHD System

**Format :** Talk at Waseda University

**Author(s) :** Xiaoding Shi (Beijing University of Chemical Technology)

**Abstract :** The barotropic compressible magnetohydrodynamic equations in a general two-dimensional bounded simply connected domain is considered here. For initial density allowed to vanish, we prove that the initial-boundary-value problem of 2D compressible MHD system admits the global strong and weak solutions without any restrictions on the size of initial data.

## [01436] Inviscid Limit Problem of radially symmetric stationary solutions for compressible Navier-Stokes equation

**Format :** Talk at Waseda University

**Author(s) :** Itsuko Hashimoto (kanazawa university)Akitaka Matsumura (Osaka university)

**Abstract :** The present paper is concerned with an inviscid limit problem of radially symmetric stationary solutions for an exterior problem in  $R^n$  ( $n \geq 2$ ) to compressible Navier-Stokes equation, describing the motion of viscous barotropic gas without external forces, where boundary and far field data are prescribed. For both inflow and outflow problems, the inviscid limit is considered in a suitably small neighborhood of the far field state. For the outflow problem, we prove the uniform convergence of the Navier-Stokes flows to the Euler flows in the inviscid limit. On the other hand, for the inflow problem, we show that the Navier-Stokes flows uniformly converge to a superposition of boundary layer solution and Euler flows in the inviscid limit. The estimates of algebraic rate toward the inviscid limit are also obtained.

00733 (2/4) : 3D @G606 [Chair: Itsuko Hashimoto]

## [01614] Convergence Rate Estimates for the Low Mach and Alfvén Number Three-Scale Singular Limit of Compressible Ideal Magnetohydrodynamics

**Format :** Talk at Waseda University

**Author(s) :** Qiangchang Ju (Institute of Applied Physics and Computational Mathematics, Beijing)

**Abstract :** Convergence rate estimates are obtained for singular limits of the compressible ideal magnetohydrodynamics equations, in which the Mach and Alfvén numbers tend to zero at different rates. The proofs use a detailed analysis of exact and approximate fast, intermediate, and slow modes together with improved estimates for the solutions and their time derivatives, and the time-integration method. This is a joint work with Bin Cheng and Steve Schochet

## [01617] Nonlinear asymptotic stability of vortex sheets with viscosity effects

**Format :** Talk at Waseda University

**Author(s) :** Qian Yuan (Chinese Academy of Sciences)

**Abstract :** In this talk, we can see that although a vortex sheet is not an asymptotic attractor for the compressible Navier-Stokes equations, a viscous profile that approximates the vortex sheet can be computed explicitly. It is shown that if the strength of vortex sheet is weak, then its associated viscous profile is asymptotically stable in the  $L^\infty$ -norm with small initial perturbations for the compressible Navier-Stokes equations.

## [01660] Time-asymptotic expansion with pointwise remainder estimates for 1D viscous compressible flow

**Format :** Talk at Waseda University

**Author(s) :** Kai Koike (Tokyo Institute of Technology)

**Abstract :** We consider solutions to 1D compressible Naiver–Stokes equations around a constant steady state. We construct a time-asymptotic expansion with pointwise remainder estimates. The leading-order term of the expansion is the well-known diffusion wave and the higher-order terms are newly introduced family of waves which we call higher-order diffusion waves. Thanks to the pointwise remainder estimates, we can show that the expansion is valid for a fixed point  $x$  and also in any  $L^p(\mathbb{R})$ -norm including the case of  $1 \leq p < 2$ . The proof is based on pointwise estimates of Green's function.

## [01694] Asymptotic stability for the two-phase Navier-Stokes equations with surface tension and gravity

**Format :** Talk at Waseda University

**Author(s) :** Hirokazu Saito (The University of Electro-Communications)

**Abstract :** We consider the motion of two immiscible, viscous, incompressible capillary fluids, fluid<sub>+</sub> and fluid<sub>-</sub>, in the presence of a uniform gravitational field acting vertically downward in  $\mathbf{R}^N$  for  $N \geq 3$ . At the initial time, fluid<sub>-</sub> occupies a half-space-like domain such as oceans of infinite depth, while the complement of its closure is filled with fluid<sub>+</sub>. The asymptotic stability of the trivial steady state is proved if fluid<sub>-</sub> is heavier than fluid<sub>+</sub>.

00733 (3/4) : 3E @G606 [Chair: Feng Xie]

## [01716] Global solutions on compressible Euler and Euler-Poisson equations

**Format :** Online Talk on Zoom

**Author(s) :** Yong Wang (Academy of Mathematics and System Sciences, CAS, China)

**Abstract :** I will talk some results on the global existence of solutions to compressible Euler and Euler-Poisson of large intial data with spherical symmetry.

## [01715] Global solutions on compressible Euler and Euler-Poisson equations

**Format :** Online Talk on Zoom

**Author(s) :** Yong Wang (Academy of Mathematics and System Sciences, CAS, China)

**Abstract :** I will talk some results on the global existence of solutions to compressible Euler and Euler-Poisson of large intial data with spherical symmetry.

## [01776] Some recent results on compressible Navier-Stokes equations

**Format :** Talk at Waseda University

**Author(s) :** Jing Li (AMSS, Chinese Academy of Sciences)

**Abstract :** We investigate the barotropic compressible Navier-Stokes equations with slip boundary conditions in a three-dimensional (3D) simply connected bounded domain, whose smooth boundary has a finite number of two-dimensional connected components. For any adiabatic exponent bigger than one, after obtaining some new estimates on boundary integrals related to the slip boundary conditions, we prove that both the weak and classical solutions to the initial-boundary-value problem of this system exist globally in time provided the initial energy is suitably small. Moreover, the density has large oscillations and contains vacuum states. Finally, it is also shown that for the classical solutions, the oscillation of the density will grow unboundedly in the long run with an exponential rate provided vacuum appears (even at a point) initially.

## [03229] Hidden structures behinds the compressible Navier-Stokes equations and its applications to the corresponding models

**Format :** Online Talk on Zoom

**Author(s) :** Xiangdi Huang (Academy of Mathematics and Systems Science)

**Abstract :** In this talk, we will review the past developments on the solutions of the compressible Navier-Stokes equations and reveal the three hidden structures which linked the weak solution to the strong one. Based on these observations, we proved the Nash's conjecture in 1958s and establish global exsistence theory for both isentropic and heat-conductive compressible Navier-Stokes equations.

Moreover, for the 3D compressible Navier-Stokes equations, we will show the existence of local weak solutions with higher regularity and local strong solutions with lower regularity. Also, we will mention the recent results on the blowup of the local strong solutions to the MHD equations in finite time and global existence of weak solutions of the compressible Navier-Stokes equations in bounded domains under Dirichlet boundary conditions.

00733 (4/4) : 4C @G606

## [00736] Modeling and Computation for Interface Dynamics in Fluids and Solids

### **Session Time & Room :**

00736 (1/2) : 2C (Aug.22, 13:20-15:00) @E708

00736 (2/2) : 2D (Aug.22, 15:30-17:10) @E708

### **Type :** Proposal of Minisymposium

**Abstract :** Interfacial phenomena are widely observed in nature and play important roles in materials science and fluid mechanics. The dynamics of the interfaces between different phases is of great interest not only because of the associated scientific questions but also due to its various applications. The different phases separated by the interfaces can be both liquids, or liquid-gas phases, or solid-gas phases, etc. Modelling and simulation of such systems is rather challenging, especially in the presence of moving contact lines. This mini-symposium will mainly focus on the mathematical modeling of interface dynamics and the development of efficient numerical methods.

**Organizer(s) :** Quan Zhao, Bo Lin

**Classification :** 65Mxx, 76Txx, 74-10, 76-10, 76Zxx

### **Minisymposium Program :**

00736 (1/2) : 2C @E708 [Chair: Bo Lin]

## [02231] Competition between viscous flow and diffusion in pinch-off dynamics

### **Format :** Talk at Waseda University

**Author(s) :** Tiezheng Qian (Hong Kong University of Science and Technology)

**Abstract :** We employ the Cahn-Hilliard-Navier-Stokes model to investigate the pinch-off dynamics of a liquid thread surrounded by a viscous fluid. A characteristic length scale is introduced to measure the competition between diffusion and viscous flow. This length scale is adjustable in the model and can approach micrometer scale for aqueous two-phase systems close to the critical point. Numerical examples are presented to show the pinch-off processes in the Stokes regime and the diffusion-dominated regime respectively.

## [02273] A phase field model of vesicle growth or shrinkage

### **Format :** Talk at Waseda University

**Author(s) :** Shuwang Li (Illinois Institute of Technology) Xiaoxia Tang (Illinois Institute of Technology) Steven Wise (University of Tennessee)

**Abstract :** We present a diffuse interface model for vesicle growth or shrinkage induced by an osmotic pressure. The model consists of an Allen-Cahn equation describing the evolution of phase field and a Cahn-Hilliard equation describing the evolution of concentration field. We establish control conditions for expanding or shrinking vesicles via a common tangent construction. Numerical experiments reveal that the model can capture the main feature of dynamics: formation of circle-like (expanding) and finger-like (shrinking) vesicles.

## [03394] A symmetrized parametric finite element method for anisotropic surface diffusion

### **Format :** Talk at Waseda University

**Author(s) :** YIFEI LI (National University of Singapore)

**Abstract :** In this talk, we introduce an energy-stable numerical scheme for 2D closed curve motion under anisotropic surface diffusion using a general anisotropic surface energy  $\gamma(n)$ . We propose a symmetric surface energy matrix  $Z_k(n)$ , derive a symmetrized variational formulation, and discretize it using an structure-preserving parametric finite element method (SP-PFEM). The SP-PFEM is proven unconditionally energy-stable under mild conditions on  $\gamma(n)$ . Finally, we report the high performance through numerical results.

## [02478] On a diffuse interface model for incompressible viscoelastic two-phase flows

**Format :** Talk at Waseda University

**Author(s) :** Yadong Liu (University of Regensburg) Dennis Trautwein (University of Regensburg)

**Abstract :** This talk concerns a diffuse interface model for the flow of two incompressible viscoelastic fluids in a bounded domain. More specifically, the fluids are assumed to be macroscopically immiscible, but with a small transition region, where the two components are partially mixed. Considering the elasticity of both components, one ends up with a coupled Oldroyd-B/Cahn–Hilliard type system, which describes the behavior of two-phase viscoelastic fluids. We prove the existence of weak solutions to the system in two dimensions for general (unmatched) mass densities, variable viscosities, different shear moduli, and a class of physically relevant and singular free energy densities that guarantee that the order parameter stays in the physically reasonable interval. The proof relies on a combination of a novel regularization of the original system and a new hybrid implicit time discretization for the regularized system together with the analysis of an Oldroyd-B type equation.

00736 (2/2) : 2D @E708

## [03198] Simulating solid-state dewetting of thin films: a phase-field approach

**Author(s) :** Wei Jiang (Professor)

**Abstract :** TBA

## [03625] Modeling and simulation for solid-state dewetting problems

**Author(s) :** Quan Zhao (University of Regensburg)

**Abstract :** Deposited thin films are unstable and could dewet to form isolated islands on the substrate in order to minimize the total surface energy. I will introduce a sharp-interface model and a diffuse-interface model for describing the dewetting of solid thin films with anisotropic surface energies. The relationship between the two models is established via the asymptotic analysis. Numerical results are presented to validate the asymptotic results and to demonstrate the anisotropic effects in the evolution.

## [02975] Modeling and Energy Stable Numerical Schemes of Network Development in Biology Gels

**Author(s) :** BOYI WANG (TU Wien)

**Abstract :** In this paper, we focus on the modeling and simulation of the network development in biological gels. A thermodynamically consistent model with homogenous Neumann or periodic boundary condition is derived based on the Rayleighian method. Two fully discrete numerical schemes are proposed to solve the problem. Energy stability is achieved at the discrete level for both schemes. Positivity-preserving property can be shown for the model with the Flory—Huggins potential at continuous and discrete level.

## [03582] The mixed finite element method applied to cavitation in incompressible nonlinear elasticity

**Author(s) :** Weijie Huang (Beijing Jiaotong University)

**Abstract :** In this talk, I will introduce a mixed finite element method for solving cavitation problem for 2D incompressible nonlinear elastic materials. The method is analytically proved to be locking-free and convergent, and it is also shown to be numerically accurate and efficient by numerical experiments. Furthermore, the newly developed accurate method enables us to find an interesting bifurcation phenomenon in multi-cavity growth.

# [00737] Numerical methods for semiconductor devices simulation and the computational lithography

**Session Time & Room :**

00737 (1/3) : 4D (Aug.24, 15:30-17:10) @E704

00737 (2/3) : 4E (Aug.24, 17:40-19:20) @E704

00737 (3/3) : 5B (Aug,25, 10:40-12:20) @E704

**Type :** Proposal of Minisymposium

**Abstract :** As the feature size of modern integrated circuits goes to nanometer-scale, the design and analysis of integrated circuits become complicated. Quantum mechanical phenomena become prominent in numerical simulations of semiconductor device. At the same time, rigorous computational lithography beyond Kirchhoff approximation becomes more important, but are too resource intensive to use for full chip applications. Efficient and accurate numerical simulation of device and lithography continues to be a challenge. We are concerned with the numerical modeling of semiconductor devices simulation and electromagnetic computation in lithography. Of particular interest to this minisymposium are recent advances on general numerical methods.

**Organizer(s) :** Junqing Chen,Tao Cui,Wenhai Lu ,Weiying Zheng**Classification :** 65N12, 65N30, 65N50**Minisymposium Program :**

00737 (1/3) : 4D @E704 [Chair: Weiying Zheng]

### [01756] Arbitrarily high order finite element methods for arbitrarily shaped domains with automatic mesh generation

**Format :** Talk at Waseda University**Author(s) :** Zhiming Chen (Chinese Academy of Sciences)

**Abstract :** We consider high-order unfitted finite element methods on Cartesian meshes with hanging nodes for elliptic interface problems. We construct a reliable algorithm to merge small interface elements with their surrounding elements to automatically generate the finite element mesh whose elements are large with respect to both domains. Numerical examples are presented to illustrate the competitive performance of the method. This talk is based on a joint work with Yong Liu.

### [01921] An iterative method for inverse lithography problem with TV regularization

**Format :** Talk at Waseda University**Author(s) :** Junqing Chen (Tsinghua University)

**Abstract :** I will introduce an alternating direction method of multipliers (ADMM) to solve an optimization problem stemming from inverse lithography. The objective functional of the optimization problem includes three terms. In the framework of ADMM method, the optimization problem is divided into several subproblems. Each of the subproblems can be solved efficiently. The convergence analysis is given. Some numerical examples are shown to illustrate the effectiveness of the method.

### [03833] A SOURCE TRANFER DOMAIN DECOMPOSITION METHOD FOR MAXWELL'S EQUATIONS

**Format :** Talk at Waseda University

**Author(s) :** TAO CUI (NCMIS, LSEC, Academy of Mathematics and Systems Science, Chinese Academy of Sciences)ZIMING WANG (School of Mathematical Sciences, University of Chinese Academy of Sciences)XUESHUANG XIANG (Qian Xuesen Laboratory of Space Technology, China Academy of Space Technology)

**Abstract :** In this paper, we develop an efficient solver for the Maxwell's equations in unbounded domain by extending the source transfer domain decomposition method (STDDM) proposed by Chen et al. Through the analysis of the fundamental solution of the Maxwell's equations, the convergence of STDDM is proved for the case of constant wave number. Numerical experiments are included, demonstrating that the proposed method can be used as an efficient preconditioner in the preconditioned GMRES method for solving the PML equation of the Maxwell's equations with constant and heterogeneous wave numbers, including an example for lithography.

### [01824] Numerical simulation for quantum transports in nano-semiconductor device

**Format :** Talk at Waseda University

**Author(s) :** Haiyan Jiang (Beijing Institute of Technology)tiao Lu (Peking University)Weitong Zhang (Peking University)

**Abstract :** We develop a new hybrid scheme for the coupled systems of quantum transport in nano-semiconductor device. Sinc-Galerkin method is used to solve the time-dependent Wigner equation numerically with the spectral convergence of the cardinal sine basis function solution of Wigner function in velocity space. A second-order semi-implicit time integration scheme is designed for the Wigner-Poisson equations (TWPEs). The numerical method is applied to study a double-barrier resonant tunneling diode (RTD). Error estimation, stability, and convergence are also

investigated concretely. Numerical experiments validate the theoretical results and present the reliability and efficiency of the proposed algorithm to simulate quantum effects.

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00737 (2/3) : 4E @E704 [Chair: Tao Cui]

## [01985] An efficient iterative scheme for the coupled Schrödinger-Poisson equations

**Format :** Talk at Waseda University

**Author(s) :** Wenhao Lu (Academy of Mathematics and Systems Science, Chinese Academy of Sciences)

**Abstract :** We propose an efficient iterative scheme for solving the coupled Schrödinger-Poisson equations in three-dimensions. In this scheme, the series of electron densities is truncated to a sum of finite terms, and only a finite number of eigenvalues are computed at each iteration step. The convergence analysis is also presented. We present numerical results that demonstrate the properties of the proposed scheme.

## [01922] Dispersion Analysis of CIP-FEM for Helmholtz Equation

**Format :** Talk at Waseda University

**Author(s) :** Haijun Wu (Nanjing University) Yu Zhou (Nanjing University)

**Abstract :** When solving the Helmholtz equation numerically, the accuracy of numerical solution deteriorates as the wave number  $k$  increases, known as ‘pollution effect’ which is directly related to the phase difference between the exact and numerical solutions, caused by the numerical dispersion. In this paper, we propose a dispersion analysis for the continuous interior penalty finite element method (CIP-FEM) and derive an explicit formula of the penalty parameter for the  $p^{\text{th}}$  order CIP-FEM on tensor product (Cartesian) meshes, with which the phase difference is reduced from  $\mathcal{O}(k(kh)^{2p})$  to  $\mathcal{O}(k(kh)^{2p+2})$ . Extensive numerical tests show that the pollution error of the CIP-FE solution is also reduced by two orders in  $kh$  with the same penalty parameter.

## [01779] Efficient Simulation Algorithm for FinFET and Gate-All-Around FET

**Format :** Talk at Waseda University

**Author(s) :** Lang Zeng (Beihang University)

**Abstract :** In this talk, our self-developed device simulator based on the framework of Mode space method will be introduced which can accurately and efficiently simulate the current characteristic of FinFET and GAA FET. In our hybrid framework, the 3D device is divided into 2D cross-sectional direction with closed boundary condition and 1D transport direction with open boundary condition. Our simulator is designed by modular concept that different physical models can be picked and combined freely.

## [01757] A finite element method for the Schrödinger-Poisson model

**Format :** Talk at Waseda University

**Author(s) :** Weiying Zheng (Academy of Mathematics and Systems Science, Chinese Academy of Sciences)

**Abstract :** We propose a finite element method for solving the coupled Schrödinger-Poisson equations in three-dimensions. The series of electron density is truncated into the sum of finite terms. Sharp estimates are proved for both the truncation error and the finite element discretization error. A robust iterative scheme is proposed to solve the nonlinearly coupled problem.

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00737 (3/3) : 5B @E704

## [00739] Inequalities and entropy with applications

**Session Time & Room :**

00739 (1/3) : 4C (Aug.24, 13:20-15:00) @A510

00739 (2/3) : 4D (Aug.24, 15:30-17:10) @A510

00739 (3/3) : 4E (Aug.24, 17:40-19:20) @A510

**Type :** Proposal of Minisymposium

**Abstract :** Mathematical inequalities are of fundamental interest due to their applications in different problems in industrial and applied mathematics. Developing a new inequality is a challenging and crucial task.

On the other hand, entropy plays a key role in theoretical physics and information theory. Investigations in entropy need new mathematical inequalities. In contrast, research in inequality provides novel characteristics of entropy and divergence. For instance, we need matrix inequalities in quantum information theory.

In this mini-symposium, our aim is to provide the recent advances, problems and ideas at the interface of mathematical inequalities and entropy with various applications.

**Organizer(s) :** Shigeru Furuichi

**Classification :** 47A63, 94A17, 81P45, 26D15, 15A45

**Minisymposium Program :**

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00739 (1/3) : 4C @A510 [Chair: Shigeru Furuichi]

## [02362] Refined Hermite-Hadamard inequalities and their applications to some $n$ variable means

**Format :** Talk at Waseda University

**Author(s) :** Kenjiro Yanagi (Josai University)

**Abstract :** It is well known that the Hermite-Hadamard inequality (called the HH inequality) refines the definition of convexity of function  $f(x)$  defined on  $[a, b]$  by using the integral of  $f(x)$  from  $a$  to  $b$ . There are many generalizations or refinements of the HH inequality. Furthermore the HH inequality has many applications to several fields of mathematics, including numerical analysis, functional analysis and operator inequality. Recently we gave several types of refined HH inequalities and obtained inequalities which were satisfied by weighted logarithmic means. In this talk, we give  $n$  variable HH inequality and apply to some  $n$  variable means. Finally we compare these means.

## [02747] Generalization of Hermite-Hadamard Mercer Inequalities for Certain Interval Valued Functions

**Format :** Talk at Waseda University

**Author(s) :** Asfand Fahad (Centre for Advanced Studies in Pure and Applied Mathematics, Bahauddin Zakariya University Multan, Pakistan)

**Abstract :** Due to its significance in economics, optimization and different fields, convex analysis theory has experienced various advancements and extensions over time. A modern development is the use of cr-convex functions to construct equivalent optimality conditions for constrained and unconstrained nonlinear optimization problems using interval-valued objective functions. By keeping in mind the relationships between convex functions and mathematical inequalities involving the convex functions, we investigated generalizations of well-known Hermite-Hadamard Mercer Inequalities for new types of cr-convex functions. We include several well-known consequences as special cases.

## [01760] Generalized spectral radius of operators and related inequalities

**Format :** Talk at Waseda University

**Author(s) :** Kais Feki (University of Monastir)

**Abstract :** In this talk, we aim to introduce the notion of the spectral radius of bounded linear operators acting on a complex Hilbert space  $\mathcal{H}$ , which are bounded with respect to the seminorm induced by a positive operator  $A$  on  $\mathcal{H}$ . We denote this new concept by  $r_A(\cdot)$ . In this presentation, several basic properties and inequalities involving  $r_A(\cdot)$  are investigated. Moreover, we study the connection between the notions of  $A$ -spectral radius and  $A$ -spectrum for  $A$ -bounded operators.

## [03970] $q$ -deformation of Böttcher-Wenzel inequality

**Format :** Talk at Waseda University

**Author(s) :** Hiromichi Ohno (Shinshu University)

**Abstract :** The Böttcher-Wenzel inequality states that the 2-norm of the commutator of matrices  $A$  and  $B$  is less than or equal to  $\sqrt{2}$  times the product of the 2-norms of  $A$  and  $B$ . In this talk, we discuss  $q$ -deformation of the Böttcher-Wenzel inequality in which the commutator is replaced by a  $q$ -commutator.

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00739 (2/3) : 4D @A510 [Chair: Hiroyuki Osaka]

**[01998] The reduced quantum relative entropy****Format :** Talk at Waseda University**Author(s) :** Frank Hansen (University of Copenhagen)**Abstract :** We introduce the notion of reduced relative quantum entropy and prove that it is convex. The result is used to give a simplified proof of a theorem of Lieb and Seiringer. We then proceed to describe an interpolation inequality between Golden-Thompson's trace inequality and Jensen's trace inequality.**[02970] On the quantum Tsallis relative entropy of real order****Format :** Talk at Waseda University**Author(s) :** Yuki Seo (Osaka Kyoiku University)**Abstract :** In 2005, Furuichi-Yanagi-Kuriyama showed 1-parameter extension of matrix trace inequalities due to Hiai-Petz, and it revealed relationships between two quantum Tsallis relative entropies. In this talk, we show matrix trace inequalities related to quantum Tsallis relative entropy of real order, and improve on Furuichi-Yanagi-Kuriyama's result by using Furuta inequality.**[02482] On log-sum inequalities****Format :** Talk at Waseda University**Author(s) :** Supriyo Dutta (National Institute of Technology Agartala)Shigeru Furuya (Nihon University)**Abstract :** I shall present our recently published article entitled "On log-sum inequalities" in Linear and Multilinear Algebra. The log-sum inequality is a fundamental tool which indicates the nonnegativity for the relative entropy. We establish a set of inequalities which are similar to the log-sum inequality. We extend these inequalities for the commutative matrices. In addition, utilizing the Lowner partial order relation and the Hansen-Pedersen theory for non-commutative positive semi-definite matrices we demonstrate several matrix-inequalities.**[02313] On certain properties of Shannon's Entropy****Format :** Talk at Waseda University**Author(s) :** Eleutherios Symeonidis (Faculty of Mathematics and Geography, Catholic University of Eichstaett-Ingolstadt)**Abstract :** Let  $P := (p_1, \dots, p_n)$  be a discrete probability distribution,  $H(P) := -\sum_{j=1}^n p_j \log p_j$  its Shannon entropy. Motivated by studies on the permutation entropy of time series of temperatures in combustion experiments we fix an integer  $k$ ,  $1 \leq k \leq n$ ,and consider the largest set  $\Delta \subset \mathbb{R}^k$  such that  $H(p_1, \dots, p_{n-k}, p_{n-k+1}, \dots, p_n) \geq H(0, \dots, 0, \frac{1}{k}, \dots, \frac{1}{k})$  ( $= \log k$ ) for all  $P$  such that  $(p_{n-k+1}, \dots, p_n) \in \Delta$ . In particular, we are interested in the smallest value of  $p$  such that  $(p, \dots, p) \in \Delta$ .

00739 (3/3) : 4E @A510 [Chair: Hiromichi Ohno]

**[02721] The permutation entropy and its applications on full-scale compartment fire data****Format :** Talk at Waseda University**Author(s) :** Flavia-Corina Mitroi-Symeonidis (Department of Applied Mathematics Academy of Economic Studies Calea Dorobanti 15-17, Sector 1 010552 Bucharest)**Abstract :** Given the sparse literature on the usefulness of the entropy in characterizing fire data, we investigate the order characteristics of the compartment fire based on experimental data. We compare known algorithms dedicated to the extraction of the underlying probabilities, checking their suitability to point out the abnormal values and structure of the time series. We claim that the permutation entropy is suitable to detect the occurrence of the flashover and unusual data in fire experiments.**[02772] A Spectral Analysis of The Correlated Random Walk****Format :** Talk at Waseda University**Author(s) :** Akihiro Narimatsu (The University of Fukuchiyama)Yusuke Ide (Nihon University)**Abstract :** In this talk, we consider a spectral analysis of the Correlated Random Walk with the isospectral coin cases. In the Szegedy's quantum walk, our method gives the arcsine law as the lower bound of the time averaged distribution.

## [05367] On a class of k-entanglement witnesses

**Format :** Talk at Waseda University

**Author(s) :** Hiroyuki Osaka (Ritsumeikan University)

**Abstract :** Recently, Yang et al. showed that each 2-positive map acting from  $\mathcal{M}_3(\mathbb{C})$  into itself is decomposable. It is equivalent to the statement that each PPT state on  $\mathbb{C}^3 \otimes \mathbb{C}^3$  has Schmidt number at most 2. It is a generalization of Perez-Horodecki criterion which states that each PPT state on  $\mathbb{C}^2 \otimes \mathbb{C}^2$  or  $\mathbb{C}^2 \otimes \mathbb{C}^3$  has Schmidt rank 1 i.e. is separable. Natural question arises whether the result of Yang et al. stays true for PPT states on  $\mathbb{C}^3 \otimes \mathbb{C}^4$ . This question can be considered also in higher dimensions. We construct a positive maps which is suspected for being a counterexample. More generally, we provide a class of positive maps  $\Phi_a$  between matrix algebras whose  $k$ -positivity properties can be easily controlled.

The estimate bounds on the parameter  $a$  are better than those derived from the spectral conditions considered by Chruściński and Kossakowski.

We found that in case where dimensions are differ by one we can give explicit analytic formula for parameter  $a$  that guarantee  $k$ -positivity.

As an application we show that  $\Phi_a$  detects  $k$ -entanglement.

This is mainly based on joint work with Tomasz Mlynik and Marcin Marciniak (arXiv:2104.14058v4, 2022).

## [03537] Violation of Bell's Inequality by Classical Correlation via Adaptive Dynamics

**Format :** Talk at Waseda University

**Author(s) :** Satoshi Iriyama (Tokyo University of Science)

**Abstract :** Ohya introduced the adaptive dynamics as subclasses of information dynamics. The notion of adaptive dynamics is helpful to find out characteristic factors in complex systems. In 2001, the chameleon effect proposed by Accardi et al. is the classical dynamics adopting that the local acts of observation may disturb local measurement, and its experimental implementation which can violate Bell's inequality was shown. In this talk, mathematical foundations of the chameleon dynamics and its applications are explained.

## [00746] Variational methods for singularities and concentration on low dimensional sets

**Session Time & Room :**

00746 (1/2) : 5B (Aug.25, 10:40-12:20) @F312

00746 (2/2) : 5C (Aug.25, 13:20-15:00) @F312

**Type :** Proposal of Minisymposium

**Abstract :** This mini-symposium focuses on recent developments in the calculus of variations with application to problems in nonlinear elasticity, plasticity, liquid crystals, and foams, with an emphasis on topological defects.

Defects play a prominent role, for example, in superfluidity, superconductivity, and plasticity. Low-energy configurations exhibit lower-dimensional concentration patterns; examples include dislocations, vortices, grain boundaries, interfaces, and phase transitions.

The aim of the mini-symposium is to bring together experts focusing on different aspects of this common big picture, to promote exchange of ideas, and identify new ways of tackling open problems.

**Organizer(s) :** Georg Dolzmann, Adriana Garroni, Lucia Scardia

**Classification :** 49J45, 35A15, 35Q74

**Minisymposium Program :**

00746 (1/2) : 5B @F312 [Chair: Lucia Scardia]

## [04293] Ginzburg-Landau with Oblique Anchoring and Boojums

**Format :** Talk at Waseda University

**Author(s) :** Lia Bronsard (McMaster University)Stan Alama (McMaster University)Dmitry Golovaty (The University of Akron)

**Abstract :** We study the Ginzburg-Landau functional with oblique angle condition via boundary penalization. We consider the singular limit and for strong anchoring strength, defects will occur in the interior, but for weaker anchoring strength all defects will occur on the boundary. These ‘boojums’ defects carry a fractional winding number and will occur in ordered pairs along the boundary. For the “light” boojums, we prove an asymptotic convergence. S. Alama, D. Golovaty, P. Mironescu are collaborators.

## [04158] Dipole removal for discrete energy minimizers

**Format :** Talk at Waseda University

**Author(s) :** Mircea Petrache (Pontificia Catolica Universidad de Chile)Adriana Garroni (University of Rome La Sapienza)Emanuele Spadaro (University of Rome La Sapienza)

**Abstract :** We consider a minimization problem for vector fields in the plane, allowing discrete vortex-like singularities, and we find conditions on the boundary datum on the boundary of a ball, under which the minimum-energy optimizer must have a single interior singularity. A consequence is that the screw dislocation energy minimizers with continuous boundary datum close enough to  $u(\theta) = \theta$  will have exactly one charge.

The approach passes by a discretized version of the problem of independent interest, connected to the initial problem via the Smirnov decomposition of 1-currents, and proved by a discussion based on the MaxFlow - MinCut theorem. The same strategy may apply to a larger class of problems with integer-degree topological singularities.

Extension of the 1-charge result are given for cases where the minimum possible number of interior singularities is larger than 1, and we give counterexamples to further extensions of the result.

## [03999] From Volterra’s dislocations to strain-gradient plasticity

**Format :** Talk at Waseda University

**Author(s) :** Raz Kupferman (The Hebrew University)Cy Maor (The Hebrew university)

**Abstract :** Dislocations, first classified by Volterra, can be viewed as generated by cut and weld procedures. It is only in the last 15 years that plasticity models have been derived rigorously as limits of models of finitely-many dislocations. In most of these works, the elemental dislocation is modeled as an “admissible” strain field, which is in a sense, a pre-assumed linearization of Volterra’s model. I will show how strain gradient plasticity are obtained from Volterra’s model.

## [01900] Harmonic dipoles in elasticity

**Format :** Talk at Waseda University

**Author(s) :** Duvan Henao (Universidad de O’Higgins)Marco Barchiesi (Università degli Studi di Trieste)Carlos Mora-Corral (Universidad Autónoma de Madrid)Rémy Rodiac (Université Paris Saclay)

**Abstract :** Malý (1993) proved that the relaxation of the neoHookean energy coincides with the neoHookean energy at diffeomorphisms, thus establishing the first existence result for neoHookean materials in 3D. We present some progress on the more explicit understanding of what deformations can fall into the weak closure of regular (injective, orientation-preserving, controlled Jacobian) maps and of the relaxed energy evaluated at deformations with singularities. For the pathological example of Conti & De Lellis (2003) we show that the singular energy is precisely twice the length of the dipole times the area of the bubble across which two portions of the elastic body which were separated in the reference configuration are now in contact in the deformed configuration. This, in turns, coincides with twice the total variation of the singular part of the derivative of the inverse map. We show that in the weak closure all maps have inverses with BV regularity, and in the axisymmetric case establish the Sobolev regularity for the first two components. In this axisymmetric case we obtain, as a lower bound for the singular energy, precise twice the variation of the singular part of the inverse. In the case of map with further SBV regularity for the inverse, we show that the singularities are dipoles, showing that the example of Conti & De Lellis is very generic.

00746 (2/2) : 5C @F312 [Chair: Adriana Garroni]

## [03156] effective geometric motions of Ginzburg–Landau equations with potentials of high-dimensional wells

**Format :** Talk at Waseda University

**Author(s) :** Yuning Liu (NYU shanghai)

**Abstract :** We study the co-dimensional one interface limit and geometric motions of parabolic Ginzburg–Landau systems with potentials of high-dimensional wells. In particular combining modulated energy methods and weak

convergence methods, we derive a sharp interface limit and the limiting harmonic heat flows in the inner and outer bulk regions segregated by the sharp interface.

## [02113] Quasistatic evolution problems for models of geomaterials coupling plasticity and damage

**Format :** Talk at Waseda University

**Author(s) :** Vito Crismale (Sapienza Università di Roma)

**Abstract :** I will discuss existence of quasistatic evolutions for a model proposed by Kazymyrenko and Marigo in 2019, which uses a suitable coupling between plasticity and damage to study the behavior of geomaterials under compression.

## [04281] Liquid crystal colloids: from the electrostatic analogy to interaction energies

**Format :** Talk at Waseda University

**Author(s) :** Raghavendra Venkatraman (Courant Institute )

**Abstract :** We discuss some recent progress on nematic liquid crystal colloids, with the goal of deriving simplified descriptions of colloidal suspensions in a liquid crystal matrix. The first half of the talk will provide justification of the so-called "electrostatic analogy" frequently used in physics (and proposed by Brochard and De Gennes in the 70s). The second half will be about interaction energies for paranematic colloids.

## [03855] Evolution of vector fields on flexible curves and surfaces

**Format :** Talk at Waseda University

**Author(s) :** Georg Dolzmann (University of Regensburg)

**Abstract :** We discuss some recent progress on a model system consisting of a flexible surface and a vector field defined on the surface in the case in which an interaction between the vector field and the conformation of the surface is present. Recent approaches towards the existence of solutions will be reviewed and short time existence will be established.

The lecture is based on joint work with Christopher Brand (Regensburg), Julia Menzel (Regensburg) and Alessandra Pluda (Pisa).

# [00747] Analysis and Numerics on Deep Learning Based Methods for Solving PDEs

**Session Time & Room :**

00747 (1/3) : 3C (Aug.23, 13:20-15:00) @F403

00747 (2/3) : 3D (Aug.23, 15:30-17:10) @F403

00747 (3/3) : 3E (Aug.23, 17:40-19:20) @F403

**Type :** Proposal of Minisymposium

**Abstract :** Various difficult PDE problems from the science and engineering now tend to be solved by numerical methods based on deep learning. This minisymposium focuses on both analytic and numerical aspects of these new methods. The speakers will talk about their recent works on the mechanism and further improvement of variational or/and physics-informed DNN-based solvers with applications to scientific computing problems.

**Organizer(s) :** Tao Luo, Zheng Ma, Zhiping Mao

**Classification :** 49N99, 65N99, Machine Learning

**Minisymposium Program :**

00747 (1/3) : 3C @F403 [Chair: Zheng Ma]

## [02903] Deep adaptive sampling for numerical PDEs

**Author(s) :** Tao Zhou (Chinese Academy of Sciences)

**Abstract :** Physics-informed neural networks (PINNs) have emerged as an effective technique for solving PDEs in a wide range of domains. It is noticed, however, the performance of PINNs can vary dramatically with different sampling procedures. For instance, a fixed set of (prior chosen) training points may fail to capture the effective solution region (especially for problems with singularities). To

overcome this issue, we present in this work an adaptive strategy, termed the failure-informed PINNs (FI-PINNs), which is inspired by the viewpoint of reliability analysis. The key idea is to define an effective failure probability based on the residual, and then, with the aim of placing more samples in the failure region, the FI-PINNs employs a failure-informed enrichment technique to adaptively add new collocation points to the training set, such that the numerical accuracy is dramatically improved. In short, similar as adaptive finite element methods, the proposed FI-PINNs adopts the failure probability as the posterior error indicator to generate new training points. We prove rigorous error bounds of FI-PINNs and illustrate its performance through several problems.

## [03007] Deep Learning for PDEs: Domain Decomposition and Adaptivity

**Author(s)** : Qifeng Liao (ShanghaiTech University)

**Abstract** : Deep learning methods currently gain a lot of interest for solving partial differential equations (PDEs). However, significant challenges still exist for these new methods to achieve high accuracy, which include properly defining loss functions and choosing effective collocation points and network structures. In our work, we propose domain decomposition and adaptive procedures to improve the accuracy and efficiency of deep learning based methods.

## [03091] Bridging Traditional and Machine Learning-based Algorithms for Solving PDEs: The Random Feature Method

**Author(s)** : JINGRUN CHEN (University of Science and Technology of China)XURONG CHI (University of University of Science and Technology of China Science and Technology of China)WEINAN E (AI for Science Institute, Beijing and Center for Machine Learning Research and School of Mathematical Sciences, Peking University)ZHOUWANG YANG (School of Mathematical Sciences, University of Science and Technology of China)

**Abstract** : One of the oldest and most studied subject in scientific computing is algorithms for solving partial differential equations (PDEs). A long list of numerical methods have been proposed and successfully used for various applications. In recent years, deep learning methods have shown their superiority for highdimensional PDEs where traditional methods fail. However, for low dimensional problems, it remains unclear whether these methods have a real advantage over traditional algorithms as a direct solver. In this work, we propose the random feature method (RFM) for solving PDEs, a natural bridge between traditional and machine learning-based algorithms. RFM is based on a combination of well-known ideas: 1. representation of the approximate solution using random feature functions; 2. collocation method to take care of the PDE; 3. penalty method to treat the boundary conditions, which allows us to treat the boundary condition and the PDE in the same footing. We find it crucial to add several additional components including multi-scale representatio and adaptive weight rescaling in the loss function. We demonstrate that the method exhibits spectral accuracy and can compete with traditional solvers in terms of both accuracy and efficiency. In addition, we find that RFM is particularly suited for problems with complex geometry, where both traditional and machine learning-based algorithms encounter difficulties.

## [03011] On deep learning techniques for solving convection-dominated convection-diffusion equations

**Author(s)** : Derk Frerichs-Mihov (Weierstrass Institute for Applied Analysis and Stochastics)Linus Henning (Free University of Berlin)Derk Frerichs-Mihov (Weierstrass Institute for Applied Analysis and Stochastics / Free University of Berlin)

**Abstract** : Convection-diffusion equations model the distribution of a scalar quantity in fluids, e.g., the concentration of drugs in blood. Many classical numerical methods produce unphysical values in practical applications when convection is

much stronger than diffusion ([1,2]).

In the last decades, the popularity of deep learning methods has risen sharply due to many success stories, e.g., ([3,4]). This talk brings together deep learning techniques and convection-diffusion equations. It shows challenges and proposes solutions to overcome them.

([1]) Augustin, M., Caiazzo, A., John, V. et al. An assessment of discretizations for convection-dominated convection-diffusion equations. Computer Methods in Applied Mechanics and Engineering, 200(47- 48), pp. 3395–3409, 2011, <https://www.doi.org/10.1016/j.cma.2011.08.012>

([2]) Frerichs, D. and John, V. On reducing spurious oscillations in discontinuous Galerkin (DG) methods for steady-state convection-diffusion equations. Journal of Computational and Applied Mathematics, 393, pp. 113487/1–113487/20, 2021, <https://www.doi.org/10.1016/j.cam.2021.113487>

([3]) Raissi, M., Perdikaris, P. and Karniadakis, G. E. Physics Informed Deep Learning (Part I): Data-driven Solutions of Nonlinear Partial Differential Equations. ArXiv, arXiv:1711.10561v1, 2017, <https://www.doi.org/10.48550/arXiv.1711.10561>

61

([4]) Karniadakis, G. E., Kevrekidis, I. G., Lu, L. et al. Physics-informed machine learning. Nature Reviews Physics, 3, pp. 422440, 2021, <https://www.doi.org/10.1038/s42254-021-00314-5>

**[04381] Learning Functional Priors and Posteriors from Data and Physics**

**Author(s)** : Xuhui Meng (Huazhong University of Science and Technology)

**Abstract** : We develop a new Bayesian framework based on deep generative models to quantify uncertainties arising from both noisy and gappy data in predictions of physics-informed neural networks (PINNs) as well as deep operator networks (DeepONets). We test the proposed method for (1) forward/inverse PDE problems; (2) PDE-agnostic physical problems, e.g., 100-dimensional Darcy problem. The results demonstrate that the proposed approach can provide accurate predictions as well as uncertainties given limited and noisy data.

**[03134] AI for Combustion**

**Author(s)** : Zhiqin Xu (Shanghai Jiao Tong University)

**Abstract** : The development of detailed chemistry mechanisms of hydrocarbon fuels paves the way to realistic simulations of practical combustors. However, due to chemistry stiffness, the simulation of large-size detailed mechanisms become forbiddingly expensive, especially for very large-scale simulation. In this talk, I will introduce a deep learning based model reduction method for simplifying chemical kinetics. We also use a deep learning based method to overcome the limitation of using small step-size in simulating the combustion ODE systems.

**[03476] DOSnet as a Non-Black-Box PDE Solver: When Deep Learning Meets Operator Splitting**

**Author(s)** : Yuan Lan (Huawei Theory Lab)Zhen Li (Huawei Theory Lab)Jie Sun (Huawei Theory Lab)Yang Xiang (Hong Kong University of Science and Technology)

**Abstract** : Deep neural networks (DNNs) recently emerged as a promising tool for analyzing and solving complex differential equations arising in science and engineering applications. Alternative to traditional numerical schemes, learning-based solvers utilize the representation power of DNNs to approximate the input-output relations in an automated manner. However, the lack of physics-in-the-loop often makes it difficult to construct a neural network solver that simultaneously achieves high accuracy, low computational burden, and interpretability. In this work, focusing on a class of evolutionary PDEs characterized by decomposable operators, we show that the classical “operator splitting” technique can be adapted to design neural network architectures. This gives rise to a learning-based PDE solver, which we name Deep Operator-Splitting Network (DOSnet). Such non-black-box network design is constructed from the physical rules and operators governing the underlying dynamics, and is more efficient and flexible than the classical numerical schemes and standard DNNs. To demonstrate the advantages of our new AI-enhanced PDE solver, we train and validate it on several types of operator-decomposable differential equations. We also apply DOSnet to nonlinear Schrödinger equations which have important applications in the signal processing for modern optical fiber transmission systems, and experimental results show that our model has better accuracy and lower computational complexity than numerical schemes and the baseline DNNs.

**[04359] Residual Minimization for PDEs: Failure of PINN and Implicit Bias**

**Author(s)** : Qixuan Zhou (Shanghai Jiao Tong University)Tao Luo (Shanghai Jiao Tong University)

**Abstract** : In this talk, we discuss the performance of PINN methods for problems with discontinuities. For linear elliptic PDEs with discontinuous coefficients, we present by experiments that PINN cannot approximate the true solution. We then prove this by introducing a modified equation. And we point out there is still some pattern behind this failure, which is a type of implicit bias. Finally, we will extend some of these results to quasilinear elliptic equations and systems.

00747 (3/3) : 3E @F403 [Chair: Tao Luo]

**[03475] Feature Flow Regularization: Improving Structured Sparsity in Deep Neural Networks**

**Author(s)** : YUE WU (The Hong Kong University of Science and Technology)YUAN LAN (The Hong Kong University of Science and Technology)Luchan Zhang (Shenzhen University)Yang Xiang (Hong Kong University of Science and Technology)

**Abstract** : Pruning is a model compression method that removes redundant parameters and accelerates the inference speed of deep neural networks while maintaining accuracy. We propose a regularization strategy from a new perspective of evolution of features. We propose feature flow regularization (FFR) to penalize the length and total absolute curvature of the trajectories, which implicitly increases the structured sparsity of the parameters. The principle is that short and straight trajectories will lead to an efficient network.

## [04428] Asymptotic-Preserving Neural Networks for Multiscale Time-Dependent Linear Transport Equations

**Author(s)** : Shi Jin (Shanghai Jiao Tong University)Zheng Ma (Shanghai Jiao Tong University)Keke Wu (Shanghai Jiao Tong University)

**Abstract** : In this paper we develop a neural network for the numerical simulation of time-dependent linear transport equations with diffusive scaling and uncertainties. The goal of the network is to resolve the computational challenges of curse-of-dimensionality and multiple scales of the problem. We first show that a standard Physics-Informed Neural Network (PINN) fails to capture the multiscale nature of the problem, hence justifies the need to use Asymptotic-Preserving Neural Networks (APNNs). We show that not all classical AP formulations are directly fit for the neural network approach. We construct a micro-macro decomposition based neural network, and also build in a mass conservation mechanism into the loss function, in order to capture the dynamic and multiscale nature of the solutions. Numerical examples are used to demonstrate the effectiveness of this APNNs.

## [00749] Recent Advances on Preconditioners and Fast Solvers for Nonlinear PDEs

**Session Time & Room :**

00749 (1/3) : 1C (Aug.21, 13:20-15:00) @E703

00749 (2/3) : 1D (Aug.21, 15:30-17:10) @E703

00749 (3/3) : 1E (Aug.21, 17:40-19:20) @E703

**Type** : Proposal of Minisymposium

**Abstract** : Numerical methods for solving nonlinear PDEs are at the heart of many scientific applications in physics, engineering, and biology. Recent advances in developing preconditioners and fast solvers bring significant improvement to the robustness and efficiency of numerical methods for nonlinear PDEs. A variety of novel techniques have been introduced such as nonlinear preconditioning, model order reduction, multiscale methods, heterogeneous computing, and machine learning. This minisymposium is to encourage communication among experts in these fields to discuss cutting-edge topics of numerical methods for nonlinear PDEs and their applications.

**Organizer(s)** : Xiao-Chuan Cai, Rongliang Chen, Li Luo

**Classification** : 65M55, 65M22, 65F08, 65Y05, 49M15

**Minisymposium Program :**

00749 (1/3) : 1C @E703 [Chair: Xiao-Chuan Cai]

## [04011] Nonlinear FETI-DP domain decomposition methods combined with deep learning

**Format** : Talk at Waseda University

**Author(s)** : Axel Klawonn (University of Cologne)Martin Läser (University of Cologne)Janine Weber (University of Cologne)

**Abstract** : In nonlinear-FETI-DP domain decomposition methods the choice of the nonlinear elimination set and of the coarse space have a huge impact on the nonlinear and linear convergence behavior. In this talk, we will show new results combining recently developed approaches for the adaptive choice of the nonlinear elimination set with adaptive coarse spaces. Additionally, we will discuss approaches to improve the computational efficiency and nonlinear convergence by enhancing Nonlinear-FETI-DP with techniques from machine learning.

## [03539] A quasi-Newton method with a secant-like diagonal approximation of Jacobian for symmetric sparse nonlinear equations

**Format** : Talk at Waseda University

**Author(s)** : Duc Quoc Huynh (National Central University)Feng-Nan Hwang (National Central University)

**Abstract** : We propose and study a new variant of the quasi-Newton method with a secant-like diagonal approximation of Jacobian (QN-SDAJ) for solving sparse symmetric nonlinear equations (SSNEs). Such problems appear in various scientific computing applications, such as finding critical points that satisfy the first-order necessary condition of unconstrained optimization problems and numerical semilinear elliptic partial differential equations. The advantages of the proposed method are conceptually simple and easy to implement. We establish the global convergence of the proposed method in conjunction with a nonmonotone line search technique under some appropriate assumptions.

Several numerical experiments for some benchmark problems demonstrate the efficiency of QN-SDAJ, which outperforms the alternatives, including exact Newton, nonlinear conjugate gradient, and Broyden--Fletcher--Goldfarb--Shanno (BFGS) methods. In addition, the proposed method can also be used as an effective nonlinear preconditioner to enhance the robustness and speed up the convergence of BFGS, especially for test cases with large dimensions.

## [02038] Robustness and Adaptivity of Iterative Solvers

**Format :** Talk at Waseda University

**Author(s) :** Chensong Zhang (AMSS)

**Abstract :** Linear systems arising from coupled PDEs in multiphysics applications could cause robustness problems for iterative solution methods. Solving large-scale linear algebraic systems in an efficient and robust manner is a dream for many computational scientists who work on practical engineering applications. In this talk, we review some old and new techniques for improving the robustness of iterative solvers for large-scale sparse linear equations. In particular, we will discuss methods based on machine learning to select solver components automatically to improve overall simulation performance. Based on this algorithm selection model, a self-adaptive procedure can be derived to improve the robustness of iterative solvers.

## [01782] Generalized multiscale finite element method for highly heterogeneous compressible flow

**Format :** Talk at Waseda University

**Author(s) :** Shubin Fu (Eastern Institute for Advanced Study)Lina Zhao (City University of Hong Kong)Eric Chung (The Chinese University of Hong Kong)

**Abstract :** I will present generalized multiscale finite element method for highly heterogeneous compressible flow. We follow the major steps of the GMsFEM to construct a permeability dependent offline basis for fast coarse-grid simulation. To further increase the accuracy of the multiscale method, a residual driven online multiscale basis is added to the offline space. Rich numerical tests on typical 3D highly heterogeneous media are presented to demonstrate the impressive computational advantages of the proposed multiscale method.

00749 (2/3) : 1D @E703 [Chair: Li Luo]

## [03859] Efficient Schwarz Preconditioning Techniques for Nonlinear Problems Using FROSch

**Format :** Talk at Waseda University

**Author(s) :** Alexander Heinlein (Delft University of Technology (TU Delft))Axel Klawonn (University of Cologne)Mauro Perego (Sandia National Laboratories)Sivasankaran Rajamanickam (Sandia National Laboratories)Lea Saßmannshausen (University of Cologne)Ichitaro Yamazaki (Sandia National Laboratories)

**Abstract :** FROSch (Fast and Robust Overlapping Schwarz) is a framework for parallel Schwarz domain decomposition preconditioners in Trilinos. Due an algebraic approach, meaning that the preconditioners can be constructed from a fully assembled matrix, FROSch is applicable to a wide range of problems. This talk is focused on the application to nonlinear problems, including computational fluid dynamics and land ice simulations. Techniques for improving the efficiency and the use of GPU architectures are discussed.

## [01916] BDDC Algorithms for Oseen problems with HDG Discretizations

**Format :** Talk at Waseda University

**Author(s) :** Xuemin Tu (University of Kansas)

**Abstract :** In this talk, the balancing domain decomposition by constraints methods (BDDC) are applied to the linear system arising from the Oseen equation with the hybridizable discontinuous Galerkin (HDG) discretization.

The original system is reduced to a subdomain interface problem which is asymmetric indefinite but can be positive definite in a special subspace. Edge/face average constraints can ensure all BDDC preconditioned GMRES iterates stay in this special subspace. Some additional edge/face constraints are used to improve the convergence. When the viscosity is large and the subdomain size is small enough, the number of iterations is independent of the number of subdomains and depends only slightly on the subdomain problem size. When the viscosity is small, the convergence can deteriorate.

## [02272] Fully implicit multi-physics solver for advanced fission nuclear power plant

**Format :** Talk at Waseda University

**Author(s) :** Han Zhang (Tsinghua University)

**Abstract :** The fission nuclear reactor power plant is a multi-physics, multi-scale and multi-component coupling system, resulting in a nonlinear partial differential equation system. Fully-implicit methods, such as the Jacobian-free Newton-Krylov method and the Newton-Krylov method, are promising choices for effectively solving such complex nonlinear systems due to their super-linear convergence rate. This talk focuses on the development of fully-implicit solution method for the advanced nuclear reactor power plant, as well as its engineering application.

## [01417] Recent advances on high-performance computing algorithms for patient-specific blood flow simulations

**Format :** Talk at Waseda University

**Author(s) :** Rongliang Chen (Shenzhen Institutes of Advanced Technology Chinese Academy of Sciences)

**Abstract :** Patient-specific blood flow simulations have the potential to provide quantitative predictive tools for virtual surgery, treatment planning, and risk stratification. To accurately resolve the blood flows based on the patient-specific geometry and parameters is still a big challenge because of the complex geometry and the turbulence, and it is also important to obtain the results in a short amount of computing time so that the simulation can be used in surgery planning. In this talk, we will present some recent results of the multi-organ blood flow simulations with patient-specific geometry and parameters on a large-scale supercomputer. Several mathematical, biomechanical, and supercomputing issues will be discussed in detail. We will also report the parallel performance of the methods on a supercomputer with a large number of processors.

00749 (3/3) : 1E @E703 [Chair: Rongliang Chen]

## [01407] Nonlinear Preconditioning Strategies Based on Residual Learning for PDEs

**Format :** Talk at Waseda University

**Author(s) :** Li Luo (University of Macau)Xiao-Chuan Cai (University of Macau)

**Abstract :** We present nonlinearly preconditioned inexact Newton methods for solving highly nonlinear system of algebraic equations from the discretization of PDEs. From a large number of numerical experiments, we observe that when the inexact Newton stagnates or fails to converge, the space of residuals often contains a subspace that is difficult to resolve by Newton iteration. We introduce a learning technique to identify this subspace and then improve the convergence.

## [02019] ENO schemes with adaptive order for solving hyperbolic conservation laws

**Format :** Talk at Waseda University

**Author(s) :** Hua Shen (University of Electronic Science and Technology of China)

**Abstract :** We present a class of ENO schemes with adaptive order for solving hyperbolic conservation laws. The proposed schemes select the optimal polynomial from several candidates that are reconstructed on stencils of unequal sizes by using a novel strategy. In this way, the schemes give high-order accuracy whenever the data is smooth but avoid the Gibbs phenomenon at discontinuities.

## [03281] Energy stable schemes for gradient flows based on the DVD method

**Format :** Talk at Waseda University

**Author(s) :** Jizhu Huang (Academy of mathematics and systems science, Chinese academy sciences)

**Abstract :** In this talk, we propose a new framework to construct energy stable scheme for gradient flows based on the discrete variational derivative method. Combined with the Runge--Kutta process, we can build an arbitrary high-order and unconditionally energy stable scheme based on the discrete variational derivative method. The new energy stable scheme is implicit and leads to a large sparse nonlinear algebraic system at each time step, which can be efficiently solved by using an inexact Newton type algorithm. To avoid solving nonlinear algebraic systems, we then present a relaxed discrete variational derivative method, which can construct linear unconditionally second-order energy stable schemes. Several numerical simulations are performed to investigate the efficiency, stability, and accuracy of the newly proposed schemes.

**[01460] Scalable multilevel preconditioners for hybrid-DG discretizations of nonlinear cell-by-cell cardiac models**

**Format :** Online Talk on Zoom

**Author(s) :** Ngoc Mai Monica Huynh (University of Pavia)

**Abstract :** We present theoretical and numerical results for a scalable and quasi-optimal BDDC preconditioner for Discontinuous Galerkin discretizations of cardiac cell-by-cell models in order to approximate the discontinuous nature of cellular networks.

The resulting discrete cell-by-cell models have discontinuous global solutions across the cell boundaries, hence the proposed BDDC preconditioner is based on appropriate dual and primal spaces with additional constraints which transfer information between cells/subdomains without influencing the overall discontinuity of the global solution.

#

**[00752] Theory and efficient methods for large-scale structured optimization models**

- [01213] Augmented Lagrangian method for matrix optimization
- [02195] Determinantal point processes for sampling minibatches in SGD
- [02194] Bregman Proximal Point Algorithm Revisited: A New Inexact Version and its Inertial Variant
- [02388] On efficient and scalable computation of the nonparametric maximum likelihood estimator in mixture models

**[00753] Numerical methods for high-dimensional problems**

- [04360] An efficient stochastic particle method for high-dimensional nonlinear PDEs
- [04066] Overcoming the dynamical sign problem via adaptive particle annihilation
- [02525] A splitting Hamiltonian Monte Carlo method for efficient sampling
- [02255] Ergodicity and sharp error estimate of Stochastic Gradient Langevin Dynamics
- [04069] Multi-level Monte Carlo methods in stochastic density functional theory
- [04185] Inchworm Monte Carlo Method for Spin Chain Models in Open Quantum Systems
- [04220] A short-memory operator splitting scheme for constant-Q viscoelastic wave equation
- [04363] Solving Boltzmann equation with neural sparse representation

**[00754] Regularization models and sampling algorithms in statistics and inverse problems**

- [03567] Efficient Bernoulli Factory MCMC
- [03753] Sampling of Student's t and stable priors for edge-preserving Bayesian inversion
- [04286] Comparison of pseudo-marginal Markov chains via weak Poincaré inequalities
- [04985] CUQipy: Computational Uncertainty Quantification for Inverse Problems in Python
- [05558] Gaussian likelihoods for non-Gaussian data
- [05515] Multi-output multilevel best linear unbiased estimators via semidefinite programming
- [03923] Simulating rare events with Stein variational gradient descent

**[00760] Improving Reproducibility, Trustworthiness and Fairness in Machine Learning**

- [01736] Improving reproducibility, trustworthiness and fairness for diverse applications of machine learning
- [01850] Multi-domain & Multi-task Generalisation on Real-World Clinical Data
- [01993] Classification of datasets with imputed missing values: does imputation quality matter?
- [02088] A critical look: overly optimistic results on the TPEHGDB dataset
- [02239] Software engineering for data science
- [02265] Leakage and the reproducibility crisis in ML-based science
- [02340] ShearletX: A Mathematical Approach Towards Explainability
- [02574] A tale of two crises: COVID-19 and ML reproducibility

**[00761] Recent Advances on quadrature methods for integral equations and their applications**

- [04432] A High-Order Close Evaluation Scheme of Helmholtz Layer Potentials in 3D
- [04811] Special quadrature via line extrapolation, with application to Stokes flow
- [05076] Corrected trapezoidal rules for boundary integral methods on non-parametrized surfaces
- [03610] Quadrature errors for layer potentials near surfaces with spherical topology
- [03612] Euler-Maclaurin formulas for near-singular integrals
- [03009] Near singularity errors in boundary integrals: identification, estimation and swapping
- [04640] An adaptive discretization technique for boundary integral equations in the plane
- [05159] A fully adaptive, high-order, fast Poisson solver for complex two-dimensional geometries
- [02383] Is polynomial interpolation in the monomial basis unstable?
- [04278] A new boundary integral equation solver for problems in exteriors of open arcs
- [04717] Density interpolation methods for volume integral operators
- [05303] Recursive product integration schemes for volume potentials on irregular domains

**[00763] Long-time dynamics of numerical methods for nonlinear evolution equations**

- [03792] Bourgain techniques for error estimates at low regularity
- [01832] Improved uniform error bounds of the time-splitting methods for the long-time (nonlinear) Schrödinger equation
- [04274] A symmetric low-regularity approximation to the nonlinear Schrödinger equation
- [04742] Symmetric low regularity integrators via a forest formula
- [04423] Quantum computation of partial differential equations
- [05333] Asymptotic expansions for the linear PDEs with oscillatory input terms: Analytical form and error analysis
- [03756] A new picture on the Strang Splitting
- [05308] The role of breathers in the formation of extreme ocean waves
- [04908] Structure-preserving finite element discretization of nonlinear PDEs
- [01990] High-order mass- and energy-conserving methods for the nonlinear Schrödinger equation
- [03931] Geometric two-scale integrators for highly oscillatory system
- [03985] Structure preserving schemes for Allen-Cahn type equations

**[00766] Deep learning techniques for inverse problems and imaging**

- [03603] Deep learning-based medical image reconstruction from incomplete data
- [05360] Deep Unrolling Networks with Recurrent Momentum Acceleration
- [05368] Spatiotemporal Imaging with Diffeomorphic Optimal Transportation
- [05387] Self-supervised deep learning for imaging

**[00768] Recent Advances in Computational Tools of Scientific Machine Learning towards Digital Twins**

- [03527] Digital Twins and Machine Learning from an Inverse Problem Perspective
- [03528] Physics-guided data-driven simulations for a digital twin
- [03532] Attributing anomalies from black-box predictions
- [03536] AI Based Medical Twin System: Investigation on Focused Ultrasound Therapeutics
- [03635] Learning reduced-order operators with Bayesian inference and Gaussian processes
- [04330] Operator learning for stochastic closures of complex dynamical systems
- [05255] ClimaX: A foundation model for weather and climate

**[00774] Applications of machine learning to analyzing time-series and imaging data**

- [03788] Predicting Bladder Pressure and Contractions from Non-Invasive Time-Series Data
- [04294] Leveraging topological data analysis for parameter estimation of an agent-based model of collective motion
- [04425] Few-Shot Learning for Leaf and Vein Segmentation
- [04513] Analysis of spatial transcriptomics using deep learning and optimal transport
- [04520] Applied Machine Learning for Overhead Imagery
- [04949] Introduction to miniymposium session: Applications of machine learning to analyzing time-series and imaging data
- [05230] Reinforcement Learning in a Digital Twin Framework for the Stabilization of an Inverted Pendulum
- [05238] Solving inverse and forward problems in the water quality model by neural networks

**[00778] Analysis, Applications, and Advances in Metamaterials and Composites**

- [03353] Double-Zero-Index metamaterials
- [04938] Rigidity and Elasticity of Kirigami and Origami Metamaterials
- [03863] The macroscopic behavior of the Kagome lattice metamaterial
- [04196] Rayleigh waves in 2D extremal materials
- [04081] Large-scale metasurface design with fast direct solvers
- [04889] Relaxation of variational principles for bounding the effective operators of composites
- [04890] Bessmertryi realizations of effective tensors for metamaterial synthesis: conjectures and counterexamples
- [05015] Time domain analysis of resonant plasmonic nano-particles
- [05234] Active exterior thermal cloaking
- [04994] Imaging conductivity with thermal noise induced currents

**[00779] Advances in numerical methods for evolutionary PDEs and applications**

- [05243] Implicit-explicit time integration for thermal radiative transfer and radiation hydrodynamics
- [03444] Semi-implicit numerical methods for level set equations
- [05021] Efficient implicit methods for the Euler equations in Lagrangian coordinates
- [03910] High-order semi-implicit schemes for evolutionary partial differential equations with higher order derivatives
- [05310] Carbuncle-free, well-balanced, positivity preserving methods for the shallow water equations, with application to the circular hydraulic jump
- [04458] New highly stiff-stable schemes for linear and nonlinear parabolic equations
- [05011] Finite-differences scheme for a tensor PDE model of bionetwork formation and applications
- [04882] Asymptotic preserving scheme for ExB drift
- [03846] Efficient simulation of high-dimensional kinetic equation
- [04978] A conservative semi-Lagrangian method for inhomogeneous Boltzmann equation
- [03164] Asymptotic preserving and uniformly unconditionally stable schemes for kinetic transport equations
- [04700] High order structure preserving schemes for MHD flows in all sonic Mach numbers

**[00781] Physical and Mathematical Research on Transport on Slippery Surfaces**

- [03772] Flows through slippery tubes and annuli
- [03964] Numerical study of longitudinal flow over liquid infused surfaces
- [02965] Viscoelastic Flows through Grooved Superhydrophobic Channels
- [04260] Jeffery's paradox for the rotation of a single 'stick-slip' cylinder
- [03147] Experimental Applications of Slippery Liquid and Liquid-like-Solid Surfaces
- [03590] Drop movement on lubricant-impregnated random textures
- [05601] Asymptotic solutions for convection in longitudinal-fin heat sinks
- [02837] Inertial effects on the flow resistance of axial-groove heat pipes
- [04287] Laminar drag reduction in surfactant-contaminated superhydrophobic channels
- [04901] Hypermobilization of superhydrophobic microchannels using light
- [04001] Analysis of surface diffusion on steady "stagnant caps" of surfactant
- [04344] Slip flow enhanced by Marangoni Stresses at a superhydrophobic air-water interface

**[00782] Recent Advances on Mimetic Difference Methods**

- [01714] Fourth-order Mimetic Differential Operators Applied to the Convection-Diffusion Equation: A matrix Stability Analysis
- [01788] Discrete mollification results in mimetic difference schemes applied to the convection-diffusion-reaction equation
- [01936] Numerical Energy Conservation Mimetic Scheme For The Advection Equation
- [01939] Energy Conservation for Mimetic Scheme for Advection Equation

**[00783] PDE Eigenvalue Problems: Computational Modeling and Numerical Analysis**

- [01926] Eigenvalues in Inverse Scattering
- [01744] Inverse eigenvalue problems for inferring crystal structure from neutron scattering data
- [01689] Application of Prolate Eigensystem to Born Inverse Scattering
- [01864] Computational tools for exploring eigenvector localization
- [01877] LOWER EIGENVALUE BOUNDS FOR THE HARMONIC AND BI-HARMONIC OPERATOR
- [01904] Reduced order models for parametric PDE eigenvalue problems
- [01686] Verification of guaranteed lower eigenvalue bounds form a hybrid-high order method
- [01859] Poisson solvers for the biharmonic eigenvalue problem with the Navier boundary condition
- [01910] Why Spectral Methods are preferred in PDE Eigenvalue Problems?
- [01726] High-precision guaranteed eigenvalue bounds using higher order finite elements and graded meshes
- [01925] Comparison of guaranteed lower eigenvalue bounds with three skeletal methods
- [02081] Novel spectral methods using multivariate Muntz polynomials/functions for Schrodinger eigenvalue problems with singular potentials
- [02157] Continuity and differentiability of eigenvalues of Laplacian with respect to general domain perturbations
- [01803] GPU-accelerated high order mimetic finite difference methods for Maxwell equations and eigenproblems
- [01881] Compatible Approximation of Holomorphic Eigenvalue Problems
- [01914] The new computational method on elastic transmission eigenvalue problem

**[00785] Learning Dynamical Systems by Preserving Symmetries, Energies, and Variational Principles**

- [01395] Symplectic Model Reduction on Quadratic Manifolds
- [01373] Identification of variational principles, symmetries, and conservation laws from data
- [01597] Data-driven structure-preserving model reduction for stochastic Hamiltonian systems
- [01793] Learning video models with Lagrangian/Hamiltonian neural networks
- [02758] Structure-preserving exterior calculus for GNNs: surrogates, physics discovery, and causality

**[00787] Space Weather: Modeling, Surrogates and Uncertainty Quantification**

- [02020] Model Calibration for Ensemble CME Simulation with the SWMF
- [02101] Model reduction with data assimilation for thermospheric mass density forecasting
- [01696] Bayesian Parameter Estimation for Ambient Solar Wind Models
- [02759] A multi-fidelity boosted method with built-in uncertainty quantification and its application to geomagnetic storms prediction

**[00789] Algorithmic advances in computational quantum mechanics**

- [04860] Deterministic algorithms for the efficient evaluation of Feynman diagrams
- [04522] Quantics tensor trains meet quantum physics
- [03608] Circuit Forms of Compressed Functions and Operators with Applications
- [05166] Tensor-network sketching and many-body physics
- [03946] Analyzing Non-equilibrium Quantum Many-body Dynamics by Dynamic Mode Decomposition
- [05317] Some mathematical insights on DMET
- [04977] Efficient algorithms for Brillouin zone and frequency integration
- [04273] Extraction of resonant states in systems with defects
- [03564] Density functional theories: reformulations and regularizations
- [04839] Fine-grained parallelism is flow-based Monte Carlo algorithms
- [04906] An unambiguous and robust formulation for Wannier localization

**[00792] Recent Advances of Modeling and Computation of Moving Boundary Problems**

- [01873] Solving motions of an incompressible interface with bending in Navier-Stokes flows
- [01918] Convergence of boundary integral methods for interfacial Stokes and Darcy flow with surface tension
- [02287] A Cartesian Grid-Based Boundary Integral Method for Moving Interface Problems
- [02762] An explicit numerical method for the Cahn-Hilliard equation
- [02792] Viscous fingers in a Hele-Shaw cell under an electric field
- [02813] Computing viscoelastic and elastoplastic deformations induced by volumetric growth
- [02818] Disturbance flow generated by particles in linear viscoelastic fluids
- [02820] Mathematical Modeling and Computation of Tumor Growth
- [02821] Hydrodynamics of Tunable Janus Particles
- [02823] Sharp interface problem of Ohta-Kawasaki Model
- [02835] Phase-field modeling and simulation of controllable dendritic growth

**[00793] SIAM Student Chapter Research Presentations**

- [03324] Continuum Limit of Nonlocal Diffusion on Inhomogeneous Networks
- [03390] Computing the invariant measure of the N-vortex problem on the sphere by Hamiltonian Monte Carlo
- [03516] REGULARIZED ADAPTIVE HUBER MATRIX REGRESSION AND DISTRIBUTED LEARNING
- [03650] Optimal Contextual Bandits with Knapsacks under Realizability via Regression Oracles
- [03692] Differentially Private Confidence Interval for Extrema of Parameters
- [03749] Spherical signal processing via framelets and convolutional neural networks
- [03813] O(N) dense direct factorization with near-perfect weak scaling.
- [03907] Distributed Optimization with Imperfect Communication

- [04039] SPHERICAL FRAMELETS FROM SPHERICAL DESIGNS
- [04179] Introducing Deep Unfolding: Incorporating Prior Knowledge into Deep Learning Models
- [05002] Koopman analysis and Dynamic mode decomposition of Elementary Cellular Automata

**[00794] Mathematical Modelling and Disease**

- [01627] Transboundary management of ecological systems with applications to diseases
- [04446] Separating Populations in Flow Cytometry Experiments: A Probabilistic Approach
- [04840] Case Studies in Modeling and Optimization for Diagnostics
- [03298] Optimal Bandwidth Selection in Bio-FET Measurements

**[00795] Topological data analysis and machine learning**

- [03334] Topological Data Analysis of Spatial Systems
- [03341] Bigraded persistence barcodes and their stability
- [03617] Learning visual representation with homological labels
- [03647] Exact multi-parameter persistent homology of time-series data: Fast and variable one-dimensional reduction of multi-parameter persistence theory
- [03657] Generic transitions for flows on surfaces with or without constraints
- [04624] Topological learning for multiscale biology
- [04715] Topological Data Analysis for Biological Images and Video
- [05453] Topological data analysis of music data and AI composition
- [05456] GRIL: A 2-parameter Persistence Based Vectorization for Machine Learning
- [05457] Topological Classification of Zero Sum Games
- [05458] Topological Embedding of Brain Networks for Differentiating Temporal Lobe Epilepsy
- [05459] Barcodes and Kernels for multiparameter persistence

**[00802] Numerical Algorithms for the Eikonal Equation and Its Applications**

- [03439] Eikonal methods applied to image segmentation
- [04713] Casualty and anisotropy in the design of eikonal solvers
- [03987] Learning to Measure Distances: High Order Accurate Efficient Eikonal Solvers on Surfaces
- [03578] An Artificial Neural Network Approach for Re-distancing Implicit Surfaces
- [03777] Approximate viscosity solutions of hamilton-Jacobi equations: a review
- [04731] Eikonal equation in 3D shape reconstruction and 3D printing
- [04972] The redistancing problem using Hopf-Lax formula and its applications
- [04630] Comparison study of image-segmentation techniques by a curvature-driven flow of planes curves
- [03535] Variational methods for distance function approximation and applications
- [02323] Solving the eikonal equation utilizing mimetic methods
- [03845] Jet marching on unstructured meshes: algorithms and applications
- [03445] Regularized eikonal equation on polyhedral meshes

**[00810] Recent Developments on the Numerical Solution of Least Squares Problems**

- [01652] MinAres: An Iterative Solver for Symmetric Linear Systems
- [02064] Fast inverse LU preconditioner based on the Sherman--Morrison formula
- [01679] GMRES using pseudoinverse for range symmetric singular systems
- [02051] Solving rank deficient mixed sparse-dense linear least-squares problems by updating preconditioned iterative methods
- [02061] Preconditioners based on random sampling for solving least squares problems
- [01654] On Convergence Analysis of the Randomized Gauss-Seidel Method
- [01890] Condition numbers for the total least squares problems
- [02050] Quantum-inspired algorithm for truncated total least squares solution
- [01317] Selecting Regularization Parameters for Nuclear Norm Type Minimization Problems
- [01895] A nonconvexly regularized least squares approach for sparsity aware estimation
- [02058] Separable Quaternion Matrix Factorization
- [01543] GMRES methods for tomographic reconstruction with an unmatched back projector

**[00814] Inverse Problems for Moving Targets**

- [03803] Direct reconstruction methods for moving sources in the wave equation
- [03831] An inverse problem in mean field game from partial boundary measurement
- [02996] Factorization method for recovering moving objects with dynamic near-field data
- [04620] Imaging a moving point source from multi-frequency data measured at one and sparse observation directions  
(part I): far-field case
- [0,\pi/2]\$.

**[00815] Recent trends in continuous optimization**

- [03738] Recent developments in multiobjective fast iterative shrinkage-thresholding algorithms
- [04395] Adaptive Gradient-Based Method for Convex Optimization Problems Under Error Bounds
- [03739] Accelerated distributed proximal conjugate gradient methods for multi-agent constrained optimization problems
- [03850] Extensions of Constant Rank Qualification Constraints condition to Nonlinear Conic Programming
- [03316] Derivative-free Low Order-Value Optimization

- [04101] A Stochastic Variance Reduced Gradient using Second Order Information
- [03875] Post-Processing with Projection and Rescaling Algorithm for Symmetric Cone Programs
- [04338] Random Subspace Newton method for unconstrained non-convex optimization
- [01619] Generalized Levenberg-Marquardt method with oracle complexity bound and local convergence
- [04603] Line search methods for nonconvex optimization in deep learning
- [01615] Proximal structured quasi-Newton method for nonlinear least squares with nonsmooth regularizer
- [03538] Newton-type proximal gradient method for multi-objective optimization with composite D.C. functions
- [04582] Sharp convex exact penalty formulations in statistical signal recovery
- [02314] Accelerating nuclear-norm regularized low-rank matrix optimization through Burer-Monteiro decomposition
- [05168] The Goemans and Williamson Algorithm Extended to Fractional Cut Covering
- [01270] Solving graph equipartition SDPs on an algebraic variety
- [00819] Secure Computing: Maintaining Personal Privacy while Analyzing Data**
  - [04041] Construction of Differentially Private Summary with Homomorphic Encryption
  - [04961] Federated Learning with Differential Privacy and Secure Computing
  - [05348] Network Security and Analytics for Reliability
- [00825] Numerical Time Integration Algorithms and Software for Machine Learning**
  - [04991] The Roles of Numerical Time Integration Algorithms and Software in the Machine Learning Revolution
  - [03318] TransNet: Transferable Neural Networks for Partial Differential Equations
  - [04020] Dissipative residual layers for unsupervised implicit parameterization of data manifolds
  - [03338] Improved Parallelism and Memory Performance for Differentiating Stiff Differential Equations
- [00827] Stochastic Rounding for Reduced-Precision Arithmetic in Scientific Computing**
  - [03817] Implementation of Stochastic Rounding
  - [04133] Software Simulation of Stochastic Rounding
  - [04508] Bounds on Non-linear Errors for Variance Computation with Stochastic Rounding
  - [04837] Trace estimation via asynchronous stochastic rounding
- [00831] Randomization for Simplified Machine Learning: Random Features and Reservoir Computers**
  - [02997] Scalable Gaussian Process Regression with Quadrature-based Features
  - [03226] Advances in Time Series Analysis With Reservoir Computing
  - [03272] Error analysis of random feature neural networks for Black-Scholes-type PDEs
  - [04091] Theoretical advances for learning functions and operators with random features
  - [04530] Photonic reservoir computing with small networks
  - [04854] Latent GP-ODEs with Informative Priors
  - [04314] A Framework for Hyperparameter Optimization for Randomized Machine Learning
  - [04861] Next-Generation Reservoir Computing, and On Explaining the Surprising Success of a Random Neural Network for Forecasting Chaos
  - [05356] Minimax optimal inference of inhomogeneous diffusions
  - [05361] Nonlinear Time Series Analysis and Data Driven Forecasting: Regional Weather Prediction & Earth's Geodynamo
  - [04474] Random Features for Epidemic Prediction
- [00837] Particle Methods for Bayesian Inference**
  - [05135] Improving Ensemble Kalman Filter performance by adaptively controlling the ensemble
  - [03030] Ensemble-based gradient inference for particle methods in optimization and sampling
  - [05138] Less interaction with forward models in Langevin dynamics: Enrichment and Homotopy
  - [04703] Metropolis-adjusted interacting particle sampling
  - [05149] Computing log-densities of time-reversed diffusion processes through Hamilton-Jacobi-Bellman equations
  - [04723] Simulation of Wasserstein gradient flows with low-rank tensor methods for sampling
  - [05014] Overparameterization of Deep ResNet: Zero Loss and Mean-Field Analysis
  - [04766] Wasserstein Steepest Descent Flows for Discrepancy Flows with Riesz Kernels
  - [04729] Neural Wasserstein Gradient Flows for Discrepancies with Riesz Kernels
- [00838] Perspectives in Artificial Intelligence and Machine Learning in Materials Chemistry, 2nd edition**
  - [01431] Discovery of New Materials by Quantum Calculations and Artificial Intelligence
  - [05452] Causal analysis of materials functionality by combining topological data analysis and physical model
  - [05575] Machine learning for materials chemistry and chemical biology
  - [01449] Topological descriptor of thermal conductivity in amorphous Si
  - [05561] Fully automatized optimization of ring-opening reactions in lactone derivatives via 2-step machine learning
  - [01724] A Trial for the Realization of Material Pattern Informatics Using Interpretable AI
  - [01688] Toward Functional Polymer Informatics
  - [01335] Understanding the role of defects and disorder in polycrystalline materials
- [00840] Efficient and scalable solvers and algorithms for multiscale phenomena**
  - [02988] A multiscale preconditioner for simulating blood flows in artery with aneurysm
  - [04469] Spectral Element discretizations in cardiac electrophysiology: a matrix-free approach
  - [03783] Monolithic solution strategies for large-scale computational problems from physiology and astrophysics
  - [04869] Platform Portable Distributed Solvers and Preconditioners in Cardiac Simulations

- [03815] Overlapping Schwarz methods for Isogeometric analysis based on generalized B-splines
- [03711] Higher Order Time Integration for EMI Cardiac Electrophysiology Simulations with Nested Subset Selection and BDDC Preconditioning
- [03593] Adaptive BDDC preconditioners for 3D divergence free virtual element discretizations of the Stokes equations.
- [03487] Efficient solvers for models of personalized whole heart electromechanics
- [02611] An efficient parallel interpolation algorithm with applications to multi-physics simulation of cardiac radiofrequency ablation
- [04831] A nonlinear preconditioning strategy for solving phase-field fracture problems in a constrained minimization framework
- [04801] Multi-scale modelling and simulation: EMI models, 3D-1D transport, and DG methods
- [04846] SCALABLE SOLVERS FOR BULK-SURFACE MATERIALS UNDERGOING SPINODAL DECOMPOSITION

**[00843] Innovative numerical methods for complex PDEs**

- [01855] Accelerating nonlinear solvers with continuous data assimilation
- [01739] Unconditionally stable numerical methods for Cahn-Hilliard-Navier-Stokes-Darcy system with different densities and viscosities
- [01884] Modified exponential Rosenbrock methods to increase their accuracy
- [01971] Low Regularity Integrators for Semilinear Parabolic Equations with Maximum Bound Principles
- [02261] A tourist's guide to operator splitting
- [02294] Adaptive exponential Runge-Kutta methods for stiff PDEs
- [02660] The Dual-Wind Discontinuous Galerkin Method for Hamilton-Jacobi Equations

**[00851] Mathematics for Big Data and Artificial Intelligence: models and challenges**

- [01685] Equivariant non-expansive operators as a bridge between TDA and geometric deep learning
- [01623] a new machine learning paradigm for protein pocket detection based on Group Equivariant Non Expansive Operators
- [01528] SLiSeS: Subsampled Line Search Spectral Gradient Method for Finite Sums
- [01698] Interpretable models for large-scale tabular datasets

**[00854] Control and stabilization of PDEs: recent advances and applications**

- [02524] Quantitative rapid stabilization of some PDE models
- [02863] Generalized Fredholm-backstepping transformation
- [02944] Indirect controllability of linear constant coefficients parabolic-transport systems
- [03571] Optimal Control of Moving Sets
- [04439] On the boundary controllability of conservation laws with boundary and source controls
- [02947] Advances on structural controllability of ensembles
- [03282] Second microlocalization and optimal decay for the Bouendi-Grushin damped wave equation
- [04573] Controls on Networks: Modeling, Learning and Applications
- [03018] Stabilization of 1D evolution systems: new approaches
- [02943] Feedback stabilization and inverse problem for a nonlocal transport equation
- [04252] The controllability of a special class of coupled wave systems
- [02522] Geometry of observable sets

**[00866] BEM and related methods for advanced applications**

- [04974] Time domain boundary elements and mesh refinements
- [05091] On improving the flexibility of an IgA-BEM multi-patch code
- [04013] Solving 2D linear elastic wave equations by scalar potentials
- [04853] Time-Domain BEM for the resolution of Elastodynamic Contact Problems

**[00869] Theory, numerics and data driven methods for fluids**

- [01423] Parameter analysis in continuous data assimilation for three-dimensional Brinkman-Forchheimer-extended Darcy model
- [04819] Boundary layers for a viscous fluid in a corner domain
- [03465] Numerical schemes for various stochastic models in hydrodynamic
- [01351] Coupling of free flow and flow in porous media
- [01798] Wellposedness of stochastic PDEs arising in fluid dynamics
- [03526] Error estimates for deep learning methods in fluid dynamics
- [01243] Reconstructing external driving forces in incompressible flow via low-mode observation
- [04541] Analysis of a rotationally constrained convection model
- [04953] Estimation of parameters on the fly via nudging methods
- [04093] Uniform Boundedness of Entropy to Compressible Navier-Stokes Equations with Vacuum
- [05089] A unified framework for the analysis of accuracy and stability of a class of data assimilation methods for the Navier-Stokes equations

**[00874] Recent advances in the analysis and numerics for phase-field models**

- [02784] Existence of weak solutions to an anisotropic electrokinetic flow model
- [02502] Global existence for a singular nonlocal phase field system with inertial term
- [02824] A structure-preserving scheme for the Liu-Wu model
- [02783] Analysis of an Allen-Cahn system in two scale topology optimization

**[00876] Inverse Problems in Partial Differential Equations and Graphs**

- [04431] Geophysics and algebraic geometry
- [03655] Retrieving coupled Yang-Mills-Higgs fields
- [03095] Inverse problems for the graph Laplacian
- [03169] Quantum computing algorithms for inverse problems on graphs
- [05146] Density results in the Calderon problem
- [03644] Rellich type theorem for lattice Hamiltonians
- [04868] Continuum limits of discrete Schrödinger operators on lattices

**[00877] Mathematical and Computational Methods for Topological Materials**

- [03694] Computation of phononic crystals using the PG finite element method
- [05337] Conically degenerate spectral points of the periodic Schrödinger operator
- [02726] Frozen Gaussian sampling for wave equations
- [05595] Unfitted Computation of edge modes in photonic graphene

**[00879] Stochastic analysis in mathematical finance**

- [03804] Constrained optimal stopping under a regime-switching model
- [04565] Remarks on pathwise Itô calculus in infinite dimensions
- [03809] Systemic Risk and Overconfidence under Stochastic Environment
- [03808] Smoothness of Directed Chain Stochastic Differential Equations and Its Applications

**[00882] Geometric Shape Generation II: Design**

- [01784] Construction of discrete zero mean curvature surfaces in Euclidean and Lorentz-Minkowski spaces
- [01406] Bifurcation of the trajectory shape in self-propelled motions
- [01771] Construction of weaving structures by standard realizations with repulsive interactions
- [01581] Generation of κ-Space Curve
- [01561] The uniqueness theorem on the shape of free-form curves
- [01775] Construction of κ-Curve Using Fractional Bézier Curve
- [01764] Generation of Aesthetic Shape by Integrable Geometry
- [01613] On the relationship between mimetic discretization and discrete exterior calculus
- [01640] Quantifying the shape of data using Topological Data Analysis
- [01713] Biangular coordinates: moving forward

**[00886] Numerical methods for stochastic partial differential equations**

- [05603] Convergence Analysis of splitting up method for nonlinear filtering problem
- [04327] CLT for approximating ergodic limit of SPDEs via a full discretization
- [04355] Energy regularized approximations for stochastic logarithmic Schrödinger equation
- [05599] Density approximation for stochastic heat equation
- [03909] Space-time Discontinuous Galerkin Methods for the  $\varepsilon$ -dependent Stochastic Allen-Cahn Equation with mild noise
- [05156] Finite differences method for stochastic heat equation with singular drifts.
- [04362] Numerical schemes and related qualitative properties for degenerate PDEs driven by Lévy noise.
- [04784] Linear implicit time-stepping schemes for SPDEs with super-linearly growing coefficients

**[00888] Geometric Shape Generation I: Structures**

- [02770] Shape modeling of umbrella surfaces
- [04221] Geometrical and structural design of pseudo-geodesic gridshells
- [02774] Preliminary research on shape searching method for curved crease origami using bending deformation
- [02924] Shape design of free-form shells with specified projected membrane forces
- [05391] Singularity of Arc- and Spiral-shaped Miura-ori as Rigid-Flat-Foldable Origami Pattern
- [03876] A first-order method for large-scale eigenvalue optimization problems in topology optimization
- [03320] Recent advances on tension-compression mixed shell form-finding
- [02771] Developable surfaces with curved folds
- [02773] Variational principle for generating discrete surfaces with piecewise constant Gaussian curvatures
- [02776] Geometric shape generation of hanging membranes
- [05556] Proposal for a temporary structure with a mechanism capable of curved folding
- [05623] Topology of vibrating shapes

**[00891] Derivative-Free Optimization Theory, Methods, and Software**

- [03615] Stochastic Average Model Methods
- [01372] DFO with Transformed Objectives and a Model-based Trust-region Method
- [01341] COBYQA — A Derivative-Free Trust-Region SQP Method for Nonlinearly Constrained Optimization
- [03192] A General Blackbox Optimization Framework for Hyperparameter Optimization in Deep Learning
- [01570] PRIMA: Reference Implementation for Powell's methods with Modernization and Amelioration

**[00893] Higher Order-type Optimization Methods for Machine Learning**

- [03305] An efficient skipping BFGS algorithm with nice Hessian correction properties
- [02797] An Overview of Stochastic Quasi-Newton Methods for Large-Scale Machine Learning
- [02795] Riemannian Natural Gradient Methods
- [04755] Newton-PMR: Newton Subspace Methods with Complexity Guarantees for Non-convex Optimization

- [02799] Real-time tool path planning using deep learning for subtractive manufacturing
- [02796] NeuroPrim: An Attention-based Model for Solving NP-hard Spanning Tree Problems
- [02832] Streaming Algorithms for Maximizing the Difference of Submodular Functions
- [03350] Recursive Importance Sketching for Rank Constrained Least Squares
- [03278] A semismooth Newton stochastic proximal point algorithm with variance reduction

**[00897] Nonlinear and nonlocal models: analysis and numerics**

- [04670] Energy gap for nonlocal model
- [04387] Kacanov Iteration
- [04258] Regularity results for fractional nonlocal equation with nonstandard growth and differentiability
- [05242] BBM-type theorem for fractional Sobolev spaces with variable exponents
- [05189] Time fractional gradient flows: Theory and numerics
- [05258] Semiconvexity estimates for integro-differential equations
- [03356] Numerics and Analysis for Multi-Term Time-Fractional Burgers-Type Equation
- [04692] The Spatially Variant Spectral Fractional Laplacian: Analytical Aspects and Parameter Selection

**[00908] Machine Learning and Data-Driven Applications using Geometric Integration**

- [03459] Geometric integration in machine learning
- [03490] Application of the Kernel Method to Learning Hamiltonian Equations
- [03180] Structured neural networks and some applications
- [02911] Auxiliary Functions as Koopman Observables
- [03401] Conservative Hamiltonian Monte Carlo
- [03462] Model Reduction of Hamiltonian Systems based on Nonlinear Approximation Methods

**[00911] Sparse Linear Solvers for Computational Science at Extreme Scales**

- [02685] GMRES+AMG Navier-Stokes Pressure Projection Solvers with RAS and ORAS Smoothers
- [04144] Scalable domain decomposition solvers for cardiac reaction-diffusion cell-by-cell models
- [04198] An immersed approach to fluid-structure-contact interaction
- [04292] Adapting Patch-based Relaxation to Generalized MHD Systems Within An Algebraic Multigrid Solver
- [04535] JXPAMG: an auto-tuning parallel AMG solver for extreme-scale numerical simulations
- [04594] PSCTOOLKIT: Parallel Sparse Computation Toolkit
- [04611] Recent Developments in Two-level Schwarz Domain Decomposition Preconditioners in Trilinos
- [05152] Preparing Algebraic Multigrid Solvers in hypre for Exascale Computers

**[00913] Geometric Mechanics and Related Topics**

- [05487] Feedback Integrators for Mechanical Systems with Holonomic Constraints
- [04689] Geometric Integrators for Neural Symplectic Forms
- [04691] Structure-Preserving Learning for GENERIC systems
- [05507] A discretization of Dirac structures and Lagrange-Dirac dynamical systems
- [03436] Noether's conservation laws via the modified formal Lagrangians
- [05483] Harmonic exponential families on homogeneous spaces
- [04618] Symmetries and bifurcations of resonant periodic orbits in perturbed Rayleigh-Bénard convection
- [05475] Geometric models in hydrodynamics

**[00915] The mathematics of quantum interaction models**

- [03491] Quantum computation and its viewpoint from spectral zeta functions
- [03218] New mathematics and machine learning applications from qubits and oscillators
- [03683] Design and optimization of fault-tolerant quantum computing
- [04189] Energy spacing and time evolution for asymmetric quantum Rabi models
- [03826] The spectral problem in Hilbert spaces of analytic functions
- [03426] The weak limit of renormalized Rabi Hamiltonian
- [03971] PT-Symmetric Quantum Rabi Model
- [03421] Spectrum of the noncommutative harmonic oscillator and number theory
- [03466] On the Weyl spectral counting function of certain semiregular global systems
- [03916] On The Spectral Zeta Function Of Second Order Semiregular Non-Commutative Harmonic Oscillators

**[00917] High-dimensional regression and sampling**

- [05486] Lattice-based algorithms for multivariate function approximation
- [05565] Efficient recovery of non-periodic multivariate functions via samples
- [04593] Polynomial tractability for integrating functions with slowly decaying Fourier series
- [04266] Weighted least-squares approximation in expected  $L^2$  norm
- [05485] On the relation between adaptive and non-adaptive randomized sampling
- [05488] A multivariate Riesz basis of ReLU neural networks
- [0,1]\$
- [0,1]^d\$
- [05533] On minimizing the training set fill distance in regression
- [05514] Efficient training of Gaussian processes with tensor product structure
- [05610] Tensor decompositions for high-dimensional kernel regression
- [05481] Optimal sampling for regression: from linear to nonlinear approximation

**[00919] Recent Advances in Hybridizable Discontinuous Galerkin Methods and Applications**

- [03033] A CO interior penalty method for mth-Laplace equation
- [03873] Output-Adaptive Hybridized Discontinuous Finite Elements for Efficient Flow Computations
- [04227] Towards boundary conditions for HDG methods for direct aeroacoustic computations
- [04312] Hybrid discontinuous Galerkin methods on multiple levels
- [04456] Combining finite element space-discretizations with symplectic time-marching schemes for linear Hamiltonian systems
- [04720] Multigrid for HDG
- [04725] HDG method for elliptic interface problems and industrial application
- [04892] A CO interior penalty method for mth-Laplace equation
- [05082] Discontinuous Galerkin Methods for High Speed Flows

**[00923] PDEs and variational computational methods in image processing, analysis and classification**

- [03551] Mathematical models and computational algorithms for 3D and 4D image processing in developmental biology and medicine
- [04223] Fractional graph Laplacian for image reconstruction
- [03561] Mathematical models for segmentation of Natura 2000 habitats in NaturaSat software
- [03205] NatNet - forward-backward diffusion classification tool
- [02834] Segmentation-based tracking of macrophages in microscopy videos
- [02927] Model-aware learning for super-resolution in fluorescence microscopy
- [02833] Macrophages trajectories smoothing by evolving curves
- [02718] Limited memory restarted lp-lq minimization methods using generalized Krylov subspaces

**[00924] Calibration and Validation of Mathematical Models for Biological Systems**

- [01710] Multiscale spatiotemporal reconstruction of single-cell genomics data
- [01731] Integrating quantitative MRI with computational modeling to predict the response of breast cancers to neoadjuvant therapy
- [04716] Deep Hybrid Modeling of Neuronal Dynamics using Generative Adversarial Networks
- [03082] Gene regulatory network dynamics in single cells
- [02727] The role of bacterial chemotaxis in microbial symbiosis
- [04509] Multi-scale modelling of the uterus and the 12 Labours project
- [02752] Bayesian discovery of mechanics and signaling during collective cell migration
- [05213] PIEZO1 regulates cellular coordination during collective cell migration

**[00932] Some recent advances on time-modulated metamaterials**

- [04433] Modeling Plasmons on Graphene with Time- and Space-Dependent Properties
- [05163] Analytical and FDTD Modelling of EM Wave Interacting with Time-Varying Media
- [04583] Using Time-Varying Systems to Challenge Fundamental Limitations in Electromagnetics and Photonics
- [03155] Energy conserving temporal metasurfaces

**[00935] Applied mathematics in industry: Success stories of collaboration between academia and industry in Mexico**

- [01598] Public Transportation in Mexico
- [01632] Successful cases of mathematical applications for business
- [01653] Statistical Methods for Natural Disaster Risk Assessment
- [01743] Collaboration between SMM and mathematical professionals in the mexican industry
- [01745] P&L Attribution and Risk Management
- [01753] Building an university-based knowledge transfer network for the financial sector: The case of Fin-ML
- [01912] Applied mathematics in industry: Success stories of collaboration between academia and industry in Mexico

**[00936] Recent advances in applications for large-scale data assimilation and inverse problems.**

- [05372] Level-set parameterisations for Ensemble Kalman Inversion
- [05415] Data assimilation for estimating nonlinear dynamics in earthquakes
- [05358] Analysis of a localized ensemble Kalman-Bucy filter with sparse observations
- [05397] Edge-preserving inversion with  $\alpha$ -stable priors

**[00941] Numerical methods for Hamilton-Jacobi equations and their applications**

- [01729] HJ equations in optimizing system-level performance objectives of Evolutionary Game Theory models
- [02691] Maximizing the probability of desirable outcomes in Hamilton-Jacobi framework
- [03127] Data assimilation for the eikonal equation on a manifold
- [03171] Hamilton-Jacobi equations on graphs with applications to data depth and semi-supervised learning
- [03726] Neural networks for first order HJB equations and application to front propagation with obstacle terms
- [03517] A system of of Hamilton-Jacobi equations characterizing geodesic centroidal tessellations
- [04710] Tropical and multi-level numerical methods for solving optimal control problems
- [04939] Exploiting Hamilton-Jacobi-Bellman equations in the representation and evolution of conservative dynamics.
- [03669] Sparse-grid WENO fast sweeping methods for Eikonal equations
- [03495] Efficient high frequency wave propagation with small sampling density
- [03786] Data-Driven Learning Method for Optimal Feedback Control
- [03577] Leveraging Multi-time Hamilton-Jacobi PDEs for Certain Scientific Machine Learning Problems

**[00949] Optimal and Efficient Algorithms for Inverse Problems**

- [05576] Geometric Scattering on Measure Spaces
- [02094] Variable Projection Methods for Solving Separable Nonlinear Inverse Problems
- [03302] Doubly Noisy Kaczmarz
- [02096] Geometric Scattering on Measure Spaces
- [03055] Conditional sampling via block-triangular transport maps
- [02631] Efficient importance sampling for Bayesian inverse problems using tensor-trains
- [02317] On structured linear measurements for tensor data recovery

**[00951] Steps Toward Robust and Stable Artificial Intelligence**

- [03569] Adversarial Ink: Componentwise Backward Error Attacks on Deep Learning
- [05048] On the extended Smale's 9th problem, phase transitions in optimisation and the limits of AI
- [04061] Intrinsic dimensionality of real-life datasets in biomedicine and drug discovery
- [05037] Generalised hardness of approximation and hallucinations -- On barriers and paradoxes in AI for image reconstruction
- [03891] Stochastic Separation Theorems for making AI Safe, Adaptive, and Robust
- [05438] Advancements in Autodiff

**[00952] Numerical methods for emerging flow problems in geosciences**

- [03640] Non-stationary probabilistic tsunami hazard assessments incorporating the influence of tides and sea level rise
- [02149] A hybrid numerical method for dispersive multiphase porous media flows
- [01968] Ocean canyon dynamics modeled using Mimetic Curvilinear Coastal Ocean Model
- [01610] Hierarchical models for the numerical simulation of shallow water flows
- [02375] A stability solver for nonlinear mountain waves
- [02890] Coupling numerical solutions of NS and GFD equations for ocean flows
- [02177] A machine learning approach to phytoplankton productivity across the GoM

**[00955] Incorporating Immune System and Heterogeneous Dynamics into Infectious Disease Modeling**

- [04516] Modelling vector-borne disease dynamics and the impact of new interventions
- [04353] Hierarchical model of West Nile virus incorporating spatio-temporal environmental effects
- [04123] How genomic data can inform contact patterns in epidemiological models
- [05574] Capturing heterogeneity: Differential effects of temperature on Culex mosquito vectors
- [04150] Immunological variables as structure variables of epidemic models
- [01323] Approximations and parameter inference of stochastic models in infectious disease epidemiology
- [04927] Intelligent immunity: wet labs, fat data, and machine learning
- [03423] Why do most sexually transmitted infections not produce long-term immunity?
- [04157] Basic concepts for the Kermack and McKendrick model with individual heterogeneity
- [04524] Statistical analysis of global COVID-19 wave dynamics
- [03113] Will cross-immunity protect the community from COVID-19 variants?
- [04936] SARS-CoV-2 variant transition dynamics are associated with vaccination rates, number of co-circulating variants, and convalescent immunity

**[00957] Mathematics of thin structures**

- [04690] A simple numerical approach for elastic rods
- [04525] A homogenized bending theory for prestrained plates
- [01825] Variational Modeling of Stress-Driven Rearrangement Instabilities
- [04480] Numerical approximation of the deformation of thin plates
- [01792] A reduced model for plates arising as low energy Gamma-limit in nonlinear magnetoelasticity
- [04118] A novel dimensional reduction for the equilibrium study of inextensional material surfaces Author links open overlay panel
- [01343] Mesoscale modeling of systems of planar wedge disclinations and edge dislocations

**[00959] Numerical modeling and analysis in electromagnetic applications**

- [03708] Recent Advances in Finite Element Methods for Electromagnetic Analysis on Integrated Circuits
- [03728] Forced field continuity condition of object interface for the vector wave equation
- [03748] A three-dimensional NEGF development using finite element method in the presence of heterogeneous quantum dots
- [04959] A Moving Mesh Method for Nano-Rod Electro-Osmosis

**[00960] Hierarchical Low Rank Tensors and DNNs for High-dimensional Approximation**

- [04419] Low-rank tensor approximation of high-dimensional functions
- [03995] Parameter-dependent multigrid method using low-rank tensor formats
- [04205] Alternating nonnegative factorizations for low-rank tensor formats
- [04392] Tensor surrogates for sensitivity analysis in the presence of polymorphic uncertainties
- [02980] Weighted sparse and low-rank least squares approximation
- [04007] Iteratively Reweighted Least Squares Recovery on Tensor Networks
- [04663] Empirical Tensor Train Approximation in Optimal Control
- [05144] Dynamical low-rank approximation of Vlasov-Poisson equations on polygonal spatial domains
- [04645] Using Low-rank Tensor Formats in Neural Networks
- [03998] Adaptive Multilevel Neural Networks for parametric PDEs with Error Estimation

**[00961] Reinforcement Learning for Financial Modeling**

- [03063] Reinforcement learning for mean field games and mean field control problems, with applications to finance
- [03255] Learning Risk Aversion with Inverse Reinforcement Learning via Interactive Questioning
- [04804] Fisher-Rao Gradient Descent for Stochastic Control Problems.
- [05398] Risk Budgeting Allocation for Dynamic Risk Measures

**[00963] Nonconvex and nonsmooth optimization**

- [01977] A lifted L1 framework for sparse recovery
- [02344] A generalized formulation for group selection via ADMM
- [02395] A novel tensor regularization of nuclear over Frobenius norms for low rank tensor recovery
- [02672] Tractable continuous approximations for a constraint selection problem

**[00965] New mathematical trends in weather prediction and inverse problems**

- [03741] Gaussian Assimilation of non-Gaussian Image Data via Pre-Processing by Variational Auto-Encoder (VAE)
- [04216] Implementing local ensemble transform Kalman filter to reservoir computing for improving weather forecast
- [04315] Sparse optimization of inverse problems regularized with infimal-convolution-type functionals
- [04562] Efficient data-driven regularization for ill-posed inverse problems in imaging
- [05386] Inverse problems for nonlocal PDEs with applications to quantum optics
- [05472] Implicit Ensemble Tangent Linear Models (IETLMs) for model differentiation
- [05482] Advances in Integrating AI and Machine Learning with Data Assimilation for Weather Prediction
- [05497] Learned weakly convex regularisers in inverse problems

**[00966] Theoretical and computational advances in measure transport**

- [05226] Optimal transport map estimation in general function spaces
- [04080] TBA
- [04165] Efficient subspace modeling via transport transforms
- [04063] Conditional simulation through the data-driven optimal transport barycenter problem
- [04311] On the Monge gap and the MBO feature-sparse transport estimator.
- [05300] Simulation-Free Generative Modeling with Neural ODEs
- [04077] Diffusion Schrödinger Bridge Matching
- [05473] Diffusion Bridge Mixture Transports, Schrödinger Bridge Problems and Generative Modeling
- [05484] Neural Optimal Transport for Single-Cell Biology
- [04231] Tensor-train methods for sequential state and parameter learning in state-space models
- [04473] Tensor train approximation of deep transport maps for Bayesian inverse problems.
- [05065] Accelerated Interacting Particle Transport for Bayesian Inversion

**[00967] Stochastic Dynamical Systems and Applications in Data Science**

- [02120] Föllmer flows: contraction, sampling and generative learning
- [02122] Stochastic systems via rough path theory: theory and numerics
- [02124] Data-driven method to learn polymer dynamics
- [02123] Transition Phenomena in Non-Gaussian Stochastic Dynamical Systems
- [02126] Understanding the diffusion models by conditional expectations
- [02127] Early-warning indicator of transition time for noise-induced critical transition of Atlantic Meridional Overturning Circulation
- [02128] Solving the Non-local Fokker-Planck Equations by Physics-informed Neural Networks
- [02129] Emergent Short-range Memory in Stochastic Gradient Noise and Its Implications on Generalization
- [03377] Modeling and learning methods applied to collective motion in biology
- [03399] Neural architectures for identifying stochastic differential equations
- [03687] Deep learning framework for solving Fokker-Planck equations with low-rank separation representation

**[00969] Eigenvalue Problems in Electronic Structure Calculations**

- [04472] Recent Advances in Self-Consistent-Field Iterations for Solving Eigenvector-Dependent Nonlinear Eigenvalue Problems
- [04337] Kohn-Sham GGA Models and Their Approximations
- [04173] Model and data driven electromagnetic inverse problems with optimal transport
- [05566] Porting Quantum ESPRESSO Eigensolvers on GPUS
- [05006] An efficient LOBPCG solver for Kohn-Sham solution
- [03997] Sampling-based approaches for multimarginal optimal transport problems with Coulomb cost
- [03145] A mixed precision LOBPCG algorithm
- [04317] An extended plane wave framework for the electronic structure calculations of twisted bilayer material systems
- [04226] Grassmann Extrapolation of Density Matrices for Born–Oppenheimer Molecular Dynamics
- [04929] Applications of Atomic Cluster Expansion in Electronic Structure Calculations
- [04280] Numerical Analysis of the Operator Modification Approach for the Calculation of Band Diagrams of Crystalline Materials

**[00970] High Performance Linear Algebra Software toward Extreme Heterogeneity**

- [03921] Using the StarPU task-based runtime system for heterogeneous platforms as the core engine for a linear algebra software stack.

- [04285] A Look at the Future of High-Performance Linear Algebra with DPLASMA and PaRSEC
- [04413] Multiple- and Mixed-Precision BLAS with C++ Template
- [05194] MATTRIS: A Scalable and Performance Portable Math Library for Heterogeneous and Multi-Device Systems based on the IRIS Runtime
- [05190] Responsibly Reckless Matrix Algorithms for HPC Scientific Applications
- [04598] A scalable multi-GPU approach for solving H2-approximated dense linear systems
- [05233] Towards a Unified Micro-kernel Abstraction for GPU Linear Algebra
- [00974] Finite element complexes and multivariate splines**
  - [02331] A polytopal exterior calculus framework
  - [05349] Finite Element Complex
  - [05423] Diagram chases yielding discrete elasticity complexes
  - [03116] Nonconforming finite element exterior calculus
  - [05444] Bounds on smooth spline spaces
  - [04982] Conforming Finite Element Methods with Arbitrary Smoothness in Any Dimension
  - [03133] An algebraic framework for geometrically continuous splines
  - [05200] Multivariate spline functions on "oranges"
  - [05202] The strain Hodge Laplacian and discretisation of the incompatibility operator
  - [02874] Nonconforming finite elements for the Brinkman Problems and Quad-curl Problems on Cubical Meshes
  - [05642] Distributional finite element BGG complexes
- [00975] Data-driven methods for learning mathematical models**
  - [05503] Recent Advances in Weak Form-Based System Identification
  - [05502] Identification of variable coefficient PDEs using group projected subspace pursuit
  - [05509] How much can one learn a PDE from its solution?
  - [05246] Learning Koopman Operators that Generalize Well
- [00977] Recent advances on sparse optimization: algorithms and applications**
  - [02162] Asymptotically Consistent Linear Convergence Rate of the Randomized Sparse Kaczmarz Method
  - [02234] A difference-of-convex algorithm for sparse support vector machines in high dimensions
  - [01567] Frank-Wolfe type methods for a class of nonconvex inequality-constrained problems
- [00980] Recent Advances in Applied Mathematics including adopting machine learning and deep learning**
  - [01658] A hybrid difference method and its postprocessings for second order elliptic problems
  - [05287] Predicting Thermoelectric Material Properties using Machine Learning
  - [05338] Classification of respiratory sounds using deep learning methods
  - [05339] Interpretable Classification for Multivariate Gait Analysis
- [00981] Various Methods for the Analysis of PDEs**
  - [03982] Carleson's problem for infinitely many fermions
  - [05489] Stabilité results for the Sobolev inequality with computable constants and optimal behaviour
  - [05451] Lifespan estimate for classical damped wave equations with some initial data
  - [05511] Blow-up for the 1d cubic NLS
- [00982] Partial Differential Equations in Fluid Dynamics**
  - [04512] Two-Dimensional Riemann Problems: Transonic Shocks and Free Boundary Problems
  - [05347] Global stability of steady supersonic flow for 1D Compressible Euler system
  - [04192] Scaling limit of vortex dynamics on the filtered-Euler flow
  - [05331] Characteristic Decomposition for Hyperbolic System
  - [04072] Global Finite-Energy Solutions of the Compressible Euler-Poisson Equations for General Pressure Laws with Spherical Symmetry
  - [04789] Global-in-time quasi-neutral limit for a two-fluid Euler-Poisson system
  - [03623] A compressible two-fluid model with unequal velocities: existence and uniqueness
  - [04539] On the Stability of Outflowing Compressible Viscous Gas
  - [04434] Hyperbolic Cattaneo-Approximation of the compressible Navier-Stokes-Fourier system
  - [04767] Local regularity conditions on initial data for local energy solutions of the incompressible Navier-Stokes equations
  - [04554] Sharp non-uniqueness of weak solutions to viscous fluids
  - [05340] On controllability of the incompressible MHD system
- [00988] Treatment of infinity and finite-time singularities in differential equations**
  - [01480] Finite-time singularity and dynamics at infinity: characterization and asymptotic expansions
  - [01461] Compactification for Asymptotically Autonomous Dynamical Systems with Applications to Tipping Points.
  - [01512] Rate-induced tipping in heterogeneous reaction-diffusion systems
  - [01527] Using Geometric Singular Perturbation Theory to Understand Singular Shocks
  - [01810] Traveling wave solutions for certain 1D degenerate parabolic equation
  - [02005] Blow-up Rates for Solutions of a Quasi-Linear Parabolic Equation
  - [02492] Computation of collision and near-collision orbits in Celestial Mechanics problems.
  - [04119] Rigorous numerics for finding the monodromy of Picard-Fuchs differential equations for a family of K3 toric hypersurfaces

**[00989] Structure and dynamics in complex biological systems**

- [01956] Controlling cell fate specification system based on network structure
- [01938] An extension of the Fiedler-Mochizuki theory to time-delay systems
- [01727] Structure-based and dynamics-based control of biological network models
- [01991] Universal structural requirements for maximal robust perfect-adaptation in biomolecular networks
- [01961] Network topology determines robustness and flexibility in chemical reaction systems
- [01937] Simplifying complex chemical reaction networks
- [01907] Multistationarity conditions for polynomial systems in biology
- [02165] Global Attractor Conjecture, Persistence Conjecture, and Toric Differential Inclusions

**[00994] Mathematical modeling approach in pharmacokinetics/pharmacodynamics**

- [05562] Principles and applications of clinical pharmacology and pharmacometrics in the drug development
- [05550] Pharmacokinetic Model of Tacrolimus based on Stochastic Simulation and Estimation in Korean Adult Transplant Recipients
- [01369] Distributional approaches expressing tumor delay of the transit compartment model
- [01975] Accurate Prediction of Drug Interactions Through Cytochrome P450 Induction

**[01000] Advances in random dynamical systems and ergodic theory**

- [01338] Random dynamical systems and multiplicative ergodic theorems
- [05504] Compound Poisson Statistics for Random Dynamical Systems via Spectral Perturbation
- [01905] Entropy and pressure formulas for conditioned random dynamical systems
- [01767] Lyapunov exponents for random perturbations of coupled standard maps
- [05620] Shear-induced effects Random Dynamical Systems
- [02045] Horseshoes for a class of non-uniformly expanding random circle maps
- [05540] Continuation of attractors of random dynamical systems with bounded noise
- [05055] Noise-induced chaos and conditioned Lyapunov exponents in a random logistic map
- [01453] On the quasi-ergodicity of absorbing Markov chains with unbounded transition densities, including random logistic maps with escape
- [0,1], where  $\omega_n$  is an i. d sequence of random variables uniformly distributed in [a,b], for  $1 \leq n \leq N$  and  $a < 4$  and  $b > 4$ .

**[01003] Mathematical Modeling and Simulation in Land-Ocean Transition Zones**

- [05505] Analytical solution to the elliptic PDE of shelf wave with the relaxation of semi-geostrophic approximation
- [05568] Boundary layer dynamics of wave-current flows over cylindrical canopies
- [05325] On discrete shape gradients of boundary type for PDE-constrained shape optimizations
- [05596] An incremental SVD method for integro-differential equations: addressing storage and computational challenges
- [05546] Causal AI Ocean Learning and Prediction
- [02217] Parameterizing the baroclinic instability with an artificial potential energy term
- [05534] Two-grid Finite Element Decoupling Scheme for the Mixed Navier-Stokes/Darcy Model
- [05525] Shape Optimization of Incompressible Navier-Stokes flows with Shape Gradients
- [03963] Simulation of Droplet-laden Turbulent Channel flow by LBM and Phase field method

**[01011] Analysis and Design of Dynamical Circuits, Systems and Networks**

- [01717] Network dynamics on electric circuits and Maxwell's equations
- [01871] Design of a delayed feedback controller based on bifurcation analysis
- [02715] Nonlinear Model Order Reduction for CT Image Reconstruction
- [02712] Analysis and Design of Recurrent Neural Networks Generating Desired Sequences of Bipolar Vectors

**[01024] Multiscale modeling and simulation methods of inhomogeneity in defected systems**

- [04025] Recent progress on multiscale coupling for crystalline defects
- [02228] Mathematical perspectives in modeling microstructures in metallic materials
- [04547] A Three-Dimensional Continuum Simulation Method for Grain Boundary Motion Incorporating Dislocation Structure
- [04727] A nonlocal elasticity model for simulating the static and dynamic problems of crystalline defects in materials
- [05384] An IBVP of a model for motion of grain boundaries
- [04942] Stochastic Continuum Models for High-Entropy Alloys with Short-range Order
- [03918] GAS: A Gaussian Mixture Distribution-Based Adaptive Sampling Method for PINNs
- [05016] An Elastic Interaction-Based Loss Function in Image Segmentation and Detection
- [03366] Phase field model for self-climb of prismatic dislocation loops by vacancy pipe diffusion
- [05129] Global weak solutions to an initial-boundary value problem of a phase-field model for motion of grain boundaries

**[01028] High-order numerical methods for nonlinear PDEs**

- [05134] Error Analysis of IMEX and Time-Splitting Schemes for the Logarithmic Schrodinger's Equation
- [02750] Constructing structure-preserving schemes via Lagrange multiplier approach
- [04415] Optimal  $L^2$  error estimates of unconditionally stable FE schemes for the Cahn-Hilliard-Navier-Stokes system
- [05392] Pointwise-in-time a posteriori error control for higher-order discretizations of time-fractional parabolic equations

- [05204] An  $L^1$  mixed DG method for second-order Elliptic Equations in the Non-divergence Form
- [02310] New analysis of a mixed FEM for Ginzburg-Landau Equations
- [01989] Spectral analysis of a mixed method for linear elasticity
- [05520] A convergent algorithm for the interaction of mean curvature flow and surface diffusion
- [02942] Optimal convergence of the arbitrary Lagrangian-Eulerian second-order projection method for the Navier-Stokes equations on an evolving domain
- [03545] Exponential Spectral Method for Semilinear Subdiffusion Equations with Rough Data

**[01029] Extremal Combinatorics and Probabilistic Combinatorics**

- [03243] Turan problem for graphs from geometric shapes
- [03233] Robust linear algebra methods and some applications
- [03332] Optimal bisections of directed graphs
- [03231] Hypergraphs with infinitely many extremal constructions
- [04610] Embeddings in “random like” hypergraphs
- [03333] Spectral extremal graphs for disjoint cliques
- [03579] Co-degree threshold for rainbow perfect matchings in uniform hypergraphs
- [03715] Recent progress on non-separating subgraphs in highly connected graphs
- [04621] Spanning trees with bounded number of leaves in  $K_{1,p}$ -free graphs
- [04636] Hadwiger’s conjecture for some graphs with independence number two
- [05371] On Connectivities of Edge-Colored Graphs

**[01036] Progress in Mathematical Programming Methods and Applications**

- [05521] An efficient solver for multi-objective onshore wind farm siting and network integration
- [02270] Steepest-Edge Simplex Algorithms for Quadratic Programming
- [02259] Techniques and advances for solving MINLPs
- [02296] New MIP presolving techniques in the Cardinal Optimizer
- [05523] News from the FICO Xpress MIP Solver and Global MINLP Solver
- [03882] Realization of smart factories using MIP
- [02009] Benders’ decomposition approach for the integrated long-haul and local VRP
- [05524] Progress in Mathematical Programming Solvers from 2001 to 2020 and future Challenges

**[01037] From interacting particles to social dynamics: modelling and analysis of agent-based systems**

- [04502] Feedback loops in opinion dynamics of agent-based and mean-field models
- [03486] Bounded Confidence Models of Opinion Dynamics
- [04255] Open systems of interacting particles: a probabilistic and multiscale framework
- [04762] Branching and coalescing particles in a singular environment

**[01040] Optimization and its Applications**

- [01444] Non-Smooth Integrability Theory
- [01446] Theoretical analysis of two time-scale update rule for training GANs
- [01450] Production Prices and Walrasian Intertemporal Competitive Equilibrium Prices in a Generalized Neoclassical Production Economy
- [01982] Optimal Growth in the Two-Sector Robinson-Shinkai-Leontief Model
- [02153] On the approximate purification of mixed strategies in games with infinite action sets
- [03646] Numerical aspects of finding nonlinear production – consumption equilibrium
- [04476] Envelope theorems in Optimization

**[01043] Applications of applied mathematics towards ocean engineering and related technologies**

- [01637] Robust control design for an autonomous underwater vehicle with uncertain dynamics
- [01719] Particle swarm optimization based robust controller for autonomous underwater vehicle
- [01959] Applications of applied mathematics towards dynamic control of multi-dimensional structures
- [01807] Ship maneuvering in waves
- [01761] AuX (X = Cu, Ag) monolayers promising Thermoelectric materials
- [01770] One-Dimensional Hetero-Nanowire Fibres for high mechanical energy storage Applications
- [01763] The Li-based quaternary Heusler compound LiYPdSn: A promising thermoelectric material
- [02187] Mathematical modeling and Environmental Impact of COVID 19 pandemic
- [01894] Highly Stable Lead-Free Magnetic Perovskite semiconductors
- [02416] CFD of impingement over a curved surface by equilaterally staggered jets
- [02634] An application of the Fuzzy inference system to Seismic Damage Prediction
- [03120] The Li-based quaternary Heusler compound LiYPdSn: A promising thermoelectric material
- [03204] Structural, electronic, dynamical and thermoelectric performance of LaCoTiSn Heusler alloy

**[01050] Delay equations in mathematical biology**

- [04514] An approach to model the bird migration
- [05022] Infectious disease dynamics with delayed control on the reproduction number
- [04371] A delayed epidemic model for behavior change
- [04511] Evolution of maturation delay

**[01054] Scalable Solvers for Multiphysics Problems**

- [01909] On the Use of Algebraic Multigrid in Various Applications on High Performance Computers

- [03924] Implications of multiphysics problems in multigrid methods from a linear algebra view point
- [03818] Parallel scalable solvers for Helmholtz problems
- [02018] Reynolds-robust preconditioners for the stationary incompressible viscoresistive MHD equations
- [04232] Robust nonlinear domain decomposition methods for problems with micro-heterogeneous structures
- [05039] Immersed Mesh Methods for Coupled Multiphysics Problems
- [04600] Towards a scalable multilevel domain decomposition solver for immersed boundary finite element method
- [03836] Co-Design of Modelling and Monolithic Overlapping Schwarz Solvers in Chemo-Mechanics
- [03397] A tensor-preserving domain decomposition preconditioner for high-order implicit methods

**[01058] Recent advances in stochastic nonlinear dynamics: modeling, data analysis**

- [02085] Almost sure averaging for fast-slow stochastic differential equations via controlled rough path
- [01488] Discrete-time Approximation of Partially Observed Stochastic Optimal Control Problem
- [03981] Large deviations for a slow-fast McKean-Vlasov model with jumps
- [02182] Recent advances in stochastic nonlinear dynamics: modeling, data analysis
- [02193] Response prediction of dynamical systems with the GCM-DL method
- [02190] Complex dynamics of a conceptual airfoil structure with consideration of extreme flight conditions
- [02205] Pattern Dynamics of Higher Order Reaction-Diffusion network
- [02243] Three occurrence mechanisms of extreme events in stochastic dynamical systems
- [02092] Homogenization of the two dimensional singular polymer measure
- [0,n]:  

$$[0, \infty), \mathbb{R}). By decomposing the drift term h$$
  

$$\text{into a singular time-homogeneous and a smooth time-dependent term, we prove that } \left\{ \frac{1}{\sqrt{n}} Z^n \right\}_{n=1}^{\infty}$$
  

$$\text{converges to a Brownian motion.}$$

**[01060] Exploring Arithmetic and Data Representation Beyond the Standard in HPC**

- [01783] FP-ANR: A representation format to handle floating-point cancellation at run-time
- [01812] Precision autotuning using stochastic arithmetic
- [01839] Implementation of highly optimized multiple precision BLAS: Strassen vs. Ozaki scheme
- [03869] Accelerating 128-bit Matrix Multiplication for Applications using FPGAs
- [04191] Multiple Integer Divisions with an Invariant Dividend
- [04628] Reduced-Precision Data Representation on Sparse Matrix-Vector Multiplications
- [04862] High-performance multidimensional integration
- [04875] Introducing MPLAPACK 2.0.1: An Extension of BLAS and LAPACK for Multiple Precision Computation
- [04912] Evaluation of various arithmetic for linear algebra on GPU and FPGA
- [05094] Using quad-precision numbers for preconditioner of domain decomposition method

**[01063] Challenges in biomathematical modeling and control**

- [05271] Analyzing infectious disease dynamics: the challenge of non-stationarity
- [05319] Models of mosquito population control strategies for fighting against arboviruse

**[01064] Recent Advances on Manifold Optimization**

- [04372] Sequential optimality conditions for nonlinear optimization on Riemannian manifolds and a globally convergent augmented Lagrangian method
- [04682] Nonlinear conjugate gradient method for vector optimization on Riemannian manifolds
- [04852] Gauss-Southwell type descent methods for low-rank matrix optimization
- [03269] Min-max optimization on manifolds
- [03743] Design of Tight Minimum-Sidelobe Windows via Optimization on Oblique Manifolds
- [04008] The Bures-Wasserstein geometry of the manifold of fixed-rank positive-semidefinite matrices
- [02861] Cayley parametrization strategy for optimization over the Stiefel manifold
- [02851] Accelerated gradient methods on the Grassmann and Stiefel manifolds
- [04571] A Riemannian ADMM
- [04455] Local stochastic algorithms for Riemannian optimization
- [03649] Riemannian Interior Point Methods for Constrained Optimization on Manifolds
- [03887] Riemannian Adaptive Optimization Algorithms and Their Applications

**[01065] Mathematics and its Applications of Risk and Decision**

- [04299] Optimal reinsurance with multivariate risks and dependence uncertainty
- [04329] Irreversible consumption habit under ambiguity: Singular control and optimal G-stopping time
- [05330] On/Off Shore Currency Rate Discrepancy
- [04244] Portfolio Selection, Periodic Evaluations and Risk Taking

**[01070] PDE Based Image Processing**

- [01942] A new PDE model for Image Inpainting
- [01962] Fractional Calculus Based Approach for Retinal Blood Vessel Segmentation
- [02860] Game theoretic Approach for Image segmentation and Image restoration by using Fractional PDE
- [02862] Higher Order PDE Model for Effective Image Denoising
- [02870] A Framework for Motion Estimation with Physics-Based Constraints in Image Sequences
- [03393] On the convergence analysis of DNN for vorticity stream function formulation and application

**[01071] Recent Advances on Groebner Bases and Their Applications**

- [01758] Parametric Ideal Operations
- [01892] On the complexity of Groebner basis computation
- [01851] On Parametric Border Basis and Comprehensive Gröbner System
- [01843] Universal Analytic Gröbner bases, Tate Algebras and toward Tropical Analytic Geometry
- [01891] Criteria for Grobner bases and degenerations by structure of signatures
- [01876] On signature-based algorithm for tropical Groebner bases on Weyl algebra
- [01898] Algorithms for bivariate lexicographic Groebner bases
- [01885] An algebraic approach to factor analysis

**[01072] Data-Driven Methods in Scientific Machine Learning**

- [05116] Acceleration of multiscale solvers via adjoint operator learning
- [05635] A Stochastic MaxiIn this work, we introduce a stochastic maximum principle (SMP) approach for solving the reinforcement learning problem with the assumption that the unknum Principle Approach for Reinforcement Learning with Parameterized Environment
- [05649] A pseudo-reversible normalizing flow for stochastic dynamical systems with various initial distributions
- [05632] Flow Map Learning for Unknown Dynamical Systems: Overview, Implementation, and Benchmarks

**[01074] Approximation Theory, Approximation Methods and Applications (ATAMA)**

- [04256] Approximation Theory, Approximation Methods and Applications: an introduction
- [04857] On the quality of adaptive methods for numerical approximation
- [05019] Monte Carlo approximation of non-autonomous Julia sets
- [05151] Projection Constants for Spaces of Multivariate Polynomials
- [05170] Stable high-order randomized cubatures for integration in arbitrary dimension
- [05108] On empirical adequacy of approximations within mathematical models
- [05186] On technical considerations of velodrome track design
- [05085] Optimal scaling of radial basis function approximations
- [04984] Interpolation on the sphere using series kernels
- [05064]  $(\beta, \gamma)$ -Chebyshev functions and points

**[01077] Recent Advances on Spectral Methods and Applications**

- [04186] A positive and moment-preserving Fourier spectral method
- [03237] Efficient structure-preserving spectral methods for plasma simulations
- [04790] A deep adaptive sampling method for the approximation of PDEs
- [04098] A variable time-step scheme for Navier-Stokes equations
- [03896] Barycentric Interpolation Based on Equilibrium Potential
- [04757] Log orthogonal functions in semi-infinite intervals: approximation results and applications
- [05466] A class of efficient spectral methods and error analysis for nonlinear Hamiltonian systems

**[01081] New Trends in Education of Applied Mathematics, Industry, Technology and Knowledge Transfer**

- [02936] Applied Mathematics curriculum in the 21 st century
- [01931] An innovative experience in a Computer Engineering programme
- [04341] How the last few years have reshaped teaching First-Year mathematics
- [04591] Experiencing Mathematics: Compute. Intuit. Imagine. Create.

**[01088] Differential Equations meet Data: Scientific Machine Learning for Cardiovascular Applications**

- [04634] Scientific machine learning approaches for many-query problems in cardiovascular applications
- [04639] GPU-Parallel Cardiac Simulation
- [05161] In-silico perivascular flow and transport
- [04430] Lipschitz Stabilised Autoencoders in Parameter Identification of Dynamical Systems
- [05201] Accelerating hemodynamic predictions via machine learning
- [04443] The fibrotic kernel signature: simulation-free prediction of atrial fibrillation
- [05176] Learning Reduced-Order Models for Blood Flow Simulations Using Graph Neural Networks
- [04920] Fast and accurate reduced order modelling techniques for the simulation of blood flow dynamics
- [04420] Parameter estimation in cardiac biomechanical models based on physics-informed neural networks
- [03697] Super-resolution and denoising of 4D flow MRI via implicit neural representations

**[01098] Elucidating theoretical biology and deep learning by algebraic statistics and topology**

- [04921] Judging unlearnability from structures of deep neural networks for low dimensional inputs
- [04805] Hit and Run Sampling from the Space of Phylogenetic Trees
- [04960] Approximate Computation of Vanishing Ideals

**[01099] Physics-based and data-driven modeling for digital twins**

- [03242] Towards smart city digital twins
- [05203] Digital twins for green carbon processes
- [01503] Hierarchical modeling of electrical machines in the context of digital twins
- [04060] From physics to machine learning and back: Applications to fault diagnostics and prognostics
- [02141] Machine Learning for Scientific Discovery, with Examples in Fluid Mechanics
- [02075] Hamiltonian structure-preserving non-intrusive operator inference for predictive digital twins
- [01631] Weakly supervised learning for power grid state estimation

- [03438] Data-driven Balancing for Acoustical Systems
- [04485] Constrained Optimal Sensing for Nuclear Digital Twins
- [03365] Exploring security challenges in enhancing Digital Twins capabilities with ChatGPT
- [04925] Reduced order modelling for large-scale CFD
- [04687] Comparison of physics-based and data-driven surrogate models of a gas-bearings supported rotor

**[01107] Efficient methods for Isogeometric Analysis**

- [04261] Matrix free weighted quadrature IgA applied to heat transfer problems
- [04410] Solving boundary value problems via the Nystrom method using spline Gauss rules
- [04643] Fast computation of electromagnetic wave propagation with spline differential forms
- [04698] Isogeometric Coupling Methods for H(curl) Problems
- [05111] Efficient reduced order models for unfitted spline discretizations
- [05187] Singularity extraction and efficient numerical integration for isogeometric BEM
- [05212] Low-rank Tensor Train Methods for IGA with Multiple Patches
- [05302] An efficient solver for space-time isogeometric Galerkin methods for parabolic problems

**[01111] Mathematical and numerical analysis on blow-up phenomena**

- [01625] On the convergence order of the numerical blow-up time
- [01957] The blow-up curve for systems of semilinear wave equations
- [01774] Lifespan estimates of semilinear wave equations of derivative type with characteristic weights in one space dimension
- [01740] On degenerate blow-up profiles for the semilinear heat equation
- [03241] Collapse Versus Blowup and Global Existence in Generalized Constantin–Lax–Majda Equation with dissipation

**[01136] Advances in Variational Models and PDEs for Images**

- [03732] Algorithms for Variational Segmentation of Regions and Boundaries
- [04275] Individual Tooth Segmentation in Human Teeth Images Using Pseudo Edge-Region Obtained by Deep Neural Networks
- [05117] Joint solution of multi-task problems in imaging
- [01799] Counting Objects by Diffused Index: geometry-free and training-free approach
- [04373] A deep quasiconformal approach for topological preserving image segmentation
- [02523] Geodesic Models with Curvature Penalization for Image Analysis
- [02808] Texture edge detection via Patch consensus
- [04153] Density-equalizing map with applications
- [01712] Application of weighted TV flow to material science problems
- [04202] Rank-One Prior: Real-Time Scene Recovery
- [02233] Multispectral Image Restoration by Structured Eigendecomposition

**[01138] Advances in embedded and Eulerian methods for fluid-structure interaction**

- [05651] A fully Eulerian FSI framework: introduction
- [05652] A fully Eulerian FSI framework: numerical approach and applications
- [02558] Embedded Methods for Floating Offshore Structures
- [03927] FULLY EULERIAN MODELS FOR FLUID-STRUCTURE INTERACTION: APPLICATION TO CAPSULES

**[01140] Modelling and simulation of electro-chemo-mechanical processes in batteries and fuel cells**

- [01934] Li-Ion battery kinetics model validation of NMC 111 and Graphite
- [04354] Fluid-electrochemical-stress-coupled Simulation Method for SOFC Degradation Prediction
- [02306] Modeling and State Estimation of Lithium-Ion Batteries under Long-Term Degradation Conditions in Aerospace Application
- [02922] Simulation of Chemo-Mechanically Coupled Battery Active Particles with Mechanical Constraints
- [04773] Electro-chemical based modelling of battery cells for automotive applications.
- [02597] Analytical solution to a multilayer particle model for Li-ion cells under generic high current profiles
- [03013] Exploring non-isothermal effects in all-vanadium redox flow batteries through advanced numerical models
- [03277] A Model Framework for Lithium Ion Intercalation Cells
- [02810] Asymptotic reduction of a model for mechanical stresses in cylindrical batteries
- [05025] Microstructural resolved simulations of NVP-C electrodes for Sodium-ion batteries
- [04382] Modeling Solid Oxide Fuel Cells based on Electrode Microstructure Information
- [05164] Improving Lithium-ion Battery Models for Porous Secondary Particles: A Comparison of Homogenized and Microscopic 3D Models

**[01145] High dimensional recent computational approaches in finance and control**

- [03950] Learning to Simulate Tail-Risk Scenarios
- [04737] Learning mappings on Wasserstein space with mean-field neural networks
- [04743] Neural Optimal Stopping Boundary
- [05236] MFG-OMO: An optimization framework for mean field game
- [03993] Statistical Learning with Sublinear Regret of Propagator Models
- [04781] ROBUST UTILITY OPTIMIZATION VIA A GAN APPROACH
- [05102] Deep Learning in Portfolio Selection under Market Frictions

[05342] Machine Learning Surrogates for Parametric and Adaptive Optimal Execution

**[01149] Sparse optimization techniques and applications**

- [05057] Efficient Magnetic Resonance Imaging via Adaptive Sparse Optimization
- [05058] A new matrix factorization for sparse representation of over-determined systems
- [05060] Sparse optimization-based ERT algorithms for multiphase flows
- [05061] Hardware-friendly binary frames for sparse optimization

**[01152] Recent trends in the mathematical theory for incompressible fluids**

- [03906] Geometric structures in incompressible fluids: vortex and magnetic reconnection
- [04219] On maximally mixed equilibria of two-dimensional perfect fluid
- [03417] Quasi-periodic invariant structures in incompressible fluids
- [03123] Flows with lower dimensional dissipations
- [03363] Uniform in gravity estimates for 2D water waves
- [04740] Invariant KAM tori around annular vortex patches for 2D Euler equations
- [03663] Euler and Navier-Stokes equations. Quasi-periodic solutions and inviscid limit
- [04625] Reducibility of a class of quasi-linear wave equation on the torus
- [02208] Nonuniqueness in Law for Stochastic Hypodissipative Navier--Stokes Equations
- [02509] Restoration of well-posedness of 2D fluid dynamics equations by transport noise
- [04785] Finite-time blowup for a 3D hypo-dissipative Navier-Stokes model equation
- [05631] Nonlinear Landau damping for the Vlasov-Poisson system in the whole space around Penrose-stable equilibria

**[01158] Oblique derivative boundary volume problems - numerical methods and applications**

- [02007] The finite element method for solving the oblique derivative boundary value problems in geodesy
- [02121] Curvature and Torsion of Gravitational Plumb Lines
- [02131] The finite volume method for solving the oblique derivative BVP in geodesy
- [02887] Finite Volume Approximate Solutions of Some Oblique Derivative Boundary Value Problems and Applications

**[01161] Error-Controlled Adaptive Algorithms in Full-Order and Reduced-Order Model Simulations**

- [01786] Modeling and multigoal-oriented a posteriori error control for heated material processing using a generalized Boussinesq modell
- [04451] Error-Controlled Local Interpolation of Moment Matching Reduced Order Models for Vibroacoustics
- [04671] Advances in A Posteriori Error Estimation and Adaptive Model Order Reduction
- [05257] Stable Linear Solves in Parametric Model Order Reduction

**[01165] Adapted Wasserstein distance for robust finance**

- [05605] Adapted Wasserstein distance for model-uncertainty in finance
- [05606] Adapted Wasserstein distance between the laws of SDEs
- [05607] Adapted Wasserstein distance on the space of continuous time stochastic processes.
- [05608] On concentration of the empirical measure for general transport costs

**[01167] Recent development in mean field control and learning**

- [04658] Actor-critic learning for mean-field control in continuous time
- [04674] Mean-field singular control problem: regularity and related mean-field reflected diffusion
- [04752] A non-asymptotic perspective on mean field control
- [05079] Signature SDEs with jumps and their tractability properties
- [05419] Markov *alpha*-Potential Game
- [05421] MF-OMO: An Optimization Formulation of Mean-Field Games
- [05439] The convergence problem in mean field control

**[01168] Network based reduced-order models for forward and inverse PDE problems**

- [02869] Regularized Lippmann-Schwinger-Lanczos Algorithm for Inverse Scattering Problems in the Frequency Domain
- [04821] Can one identify damped Stieltjes string from its spectral function?
- [04751] Inverse scattering in attenuating media -- a ROM approach
- [05171] REDUCED ORDER MODELING INVERSION OF MONOSTATIC DATA IN A MULTI-SCATTERING ENVIRONMENT
- [05531] Waveform Inversion via Reduced Order Modeling
- [05544] Correlation-informed dictionary learning for imaging in complex media

**[01170] High Performance Multigrid Methods for Large-Scale Applications**

- [03275] Block-structured and hierarchical hybrid grid matrix-free multigrid solvers for CFD applications at scale
- [03867] Performance improvements of algebraic multigrid algorithms on modern system architectures
- [03020] Improving AMG Strength of Connection
- [05263] Monolithic Multigrid and Block Preconditioning for Magnetic Confinement Fusion Relevant Resistive MHD Simulations
- [03865] Combined On/Off Node Performance Model for SPMV in Multigrid
- [05232] Recent Advances in Linear Solvers for Ice Sheet Modeling
- [05118] A Matrix-Free Approach for Algebraic Multigrid for High-Order Systems
- [03319] Mixed formulations and monolithic multigrid methods for smectic-A liquid crystals

**[01174] Hypernetworks and their dynamics in theory and applications**

- [04246] Bridging between higher-order mechanisms and phenomena
- [03667] Emergent hypernetworks in weakly coupled oscillators
- [04161] Do higher-order interactions promote coexistence in diverse ecological communities?
- [04389] Hypernetworks: cluster synchronization is a higher order effect

**[01178] On the Interplay between Kinetic Theory and Quantum Dynamics**

- [04305] Emergent phenomena in an interacting Bose gas
- [05382] Fluid limits from Quantum Boltzmann equation
- [04436] An explicit coercivity estimate of the linearized quantum Boltzmann operator
- [04331] Frozen Gaussian Approximation for open quantum system
- [04798] Quantum Dynamics of Incommensurate System
- [04339] On the kinetic description of the objective molecular dynamics

**[01181] Variational methods for multi-scale dynamics**

- [04903] Controlling conservation laws: Entropy-Entropy flux pairs
- [03821] Transport problems with non linear mobilities: a particle approximation result.
- [04444] Variational convergence for irreversible population dynamics
- [03883] Mathematical modeling of structured magnesium alloys
- [04828] Variational numerical schemes for gradient flows
- [04971] Quantitative coarse-graining of Markov chains
- [04391] Variational convergence from mean-field stochastic particle systems to the exchange-driven growth model
- [05130] On time-splitting methods for gradient flows with two dissipation mechanisms
- [0,\infty[\$ and defines a gradient-flow equation.

**[01188] Recent Developments in Fluid Dynamics**

- [04609] Recent progress on singularity formation in incompressible fluids
- [04708] Gravity Unstable Muskat Bubbles
- [04950] Whitham's highest cusped wave
- [03258] On the (in)stability of smooth self-similar solutions to the compressible Euler equations
- [04242] Small scale creation for the 2D Boussinesq Equation
- [05046] On the motion of an internal wave in two-dimensional viscous flow
- [03025] Smooth imploding solutions for 3D compressible fluids
- [04870] Stability of a point charge for the Vlasov-Poisson system
- [05033] Global axisymmetric Euler flows with rotation
- [02875] On the analyticity of the Muskat equation

**[01190] Recent Advances in Modeling Complex Systems and Multiscale Problems in Mathematical Biology**

- [04951] A Spatially Averaged Model for Platelet Cohesion by vWF
- [04400] Investigating traveling waves in biophysical models of cardiac dynamics
- [05165] Modeling and Simulation of Mucin-like Polyelectrolyte Gels
- [04304] Adaptive IMEX method for fractional PDE in viscoelastic fluids
- [04322] A mathematical model of microtubule assembly and polarity in dendrites
- [04441] Parameter Estimation for Mechanistic Models of Tear Film Breakup
- [05183] Modelling Glucose Regulation: Lipotoxicity and the Progression to Type 2 Diabetes
- [04351] PIEZO1 regulates cellular coordination during collective cell migration

**[01191] Recent advances on regularity and irregularity of fluids flows**

- [03313] Singularity formation for models of fluids
- [03731] Vorticity estimates for the 3D incompressible Navier-Stokes equation
- [04943] On criticality of the Navier-Stokes diffusion
- [05062] Well-posedness of mildly regularized active scalars in Sobolev spaces
- [04347] Bounded weak solutions to the 2D quasi-geostrophic equation
- [02935] On the support of anomalous dissipation measures
- [03059] Kinetic shock profiles for the Landau equation
- [04056] On sharp-crested water waves and finite-time singularity formation
- [04796] Turbulent solutions of fluid equations
- [03868] A localized maximum principle and its application to the critical SQG on bounded domain
- [03232] Speeding up Langevin Dynamics by Mixing
- [04760] On intermittent strong Onsager conjecture

**[01195] Hyperbolic one-dimensional systems in networks: mathematical modeling and numerical approximations**

- [02382] Control of advection-diffusion equations on networks and singular limits
- [02297] A second order model of traffic with organization marker
- [02293] Limiting flow in atrial-ventricular function
- [02299] The Junction Riemann Problems under transonic scenarios: application to veins.
- [02244] Numerical and physical impact of coupling conditions for one dimensional blood flow models
- [02355] High-order fully well-balanced numerical methods for one-dimensional blood flow in networks

**[01197] Numerical linear algebra in convex and nonconvex optimization**

- [01875] Nonconvex accelerated gradient descent without parameter tuning

- [02180] Low Rank Tensor Decompositions and Approximations
- [05344] Efficient and numerically stable interior-point algorithms for convex optimization
- [01199] Recent advances of scientific computing and applications**
  - [04888] Plant virus propagation models with delay and stochasticity
  - [05157] Numerical studies to the Chaplygin gas equation
  - [05160] Fully coupled averaging with singularities.
- [01200] New Trends in Optimal Control and Their Applications**
- [01202] Analysis and modelling of human flows**
  - [03707] Recent Public Data Related with Urban Vehicle Traffic Simulation
  - [04718] Urban scale pedestrian simulation and analysis around Kobe City center
  - [02895] Potential field of human flow extracted by Hodge-Kodaira decomposition
  - [03549] Towards science of multi-scale human flow
- [01211] Generalized and non-Gaussian Tensor Decompositions**
  - [05616] Generalized Canonical Polyadic Tensor Decomposition: Algorithms and Applications
  - [05224] Recent Improvements in CP Poisson Tensor Algorithms
  - [04808] Second-order algorithms for canonical polyadic decomposition with non-least-squares cost functions
  - [05553] Efficient Algorithms and Software for Generalized Tensor Completion
  - [03326] Stochastic Mirror Descent for Low-Rank Tensor Decomposition Under Non-Euclidean Losses
  - [03666] Generalized Tucker tensor estimation: An optimal statistical and computational framework
- [01218] Challenges in single-cell data science: theory and application**
  - [03514] Resolution of the curse of dimensionality in single-cell RNA sequencing data analysis
  - [05223] Trajectory inference framework by entropic Gaussian mixture optimal transport
  - [03619] Dissecting cell identity via network inference and in-silico gene perturbation
  - [03878] Experimental guidance for discovering genetic networks from time series
  - [03512] Geometry-aware high-dimensional vector field reconstruction using Hodge decomposition
  - [03922] Reconstructing single cell dynamics on graphs
  - [04897] Deep generative models to reveal cellular level dynamics and communication
  - [03515] Functional annotation-driven unsupervised clustering for single-cell data
  - [03908] Modelling cell differentiation: from psuedo-time to energy landscape
  - [03682] Integrating data and dynamics in scRNA-seq data analysis
- [01221] FreeFEM software package for finite element modeling of PDEs**
  - [02183] Phase field crack growth simulation using IPOPT package
  - [02252] Direct factorization of indefinite matrix for constrained problem in finite element modeling
  - [02281] An easy-to-use framework for the density-based topology optimization of multiphysics systems written in FreeFEM-PETSc-ParMmg
  - [02204] Recent advances with FreeFEM in parallel and its interface to PETSc
- [01229] Cauchy problem for Deterministic and Stochastic nonlinear dispersive equations**
  - [03890] The well-posedness of the stochastic nonlinear Schrödinger equations in  $H^2$
  - [04966] Time behavior of solutions to nonlinear Schrödinger equation with a potential
  - [03584] Well-posedness for the fourth-order Schrödinger equation with third order derivative nonlinearities
  - [05020] Convergence of the intermediate long wave equation from a statistical perspective
- [01272] Interface motion and related topics**
  - [02736] Numerical computation of the Plateau problem by the method of fundamental solutions
  - [04050] Novel numerical methods for solving nonlinear evolutionary equations with application in mathematical finance optimization problems
  - [02939] Mathematical modeling of flame/smoldering front-evolution and its application
  - [04059] Multidimensional partial integro-differential equation in Bessel potential spaces with applications
  - [04426] Qualitative and numerical aspects of dynamics of diffusion and transport mechanisms on evolving curves
  - [02845] Numerical solution to a free boundary problem for the Stokes equation using the coupled complex boundary method in shape optimization settings
  - [03222] Structure-preserving numerical methods for gradient flows of planar closed curves
  - [02751] Motion of Space Curves by Binormal and Normal Curvature
- [01383] Sustainable Logistics and Transportation under Uncertain Environments**
- [01445] Deep Learning, Preconditioning, and Linear Solvers**
  - [03314] Deep Learning, Preconditioning, and Linear Solvers
  - [04332] Fourier Neural Solver for Large Sparse Linear Algebraic Systems
  - [03199] Accelerating multigrid solvers for the acoustic and elastic Helmholtz equation.
  - [03141] On learning neural operators of PDEs with interfacial jump conditions for accelerating simulations of physical systems
  - [03614] A Deep Conjugate Direction Method for Iteratively Solving Linear Systems
  - [03251] Wasserstein GAN and Transfer Learning in physics-informed neural networks
- [01494] Queues and Related Stochastic Models**
  - [02929] Strategic revenue management for discriminatory processor sharing queues

- [03027] Bounding performance of stochastic models for server virtualization in cloud computing
- [03114] Strategic behaviour of reserved customers in a queueing model with multiple reservation zones
- [02958] Analysis of time-dependent queues with generally distributed retrials
- [03351] The rational outcome of queueing games: A fixed-point iteration based approach
- [03189] Workload analysis of fluid polling models

**[01532] Recent Trends in Fluid Mechanics and its Applications**

- [01972] Global BV solution and relaxation limit for Greenberg-Klar-Rascle model
- [02450] Global Transonic Solutions of Compressible Euler-Poisson Equations in Semiconductors
- [02456] Finite Speed of Propagation of the Relativistic Landau and Boltzmann Equations
- [02865] Global Transonic Solutions of Hot-Jupiter Model for exoplanetary atmosphere

**[01545] Interplay between controllability and qualitative aspects of stochastic dynamical systems**

- [05477] Mixing via controllability
- [05602] Multi-bubble blow-ups and multi-solitons to focusing (stochastic) nonlinear Schrödinger equations
- [04445] Controllability results for a class of bilinear degenerate wave equations
- [02831] Small-time approximate controllability for nonlinear Schrödinger equations via bilinear controls
- [03022] Small-time control of bilinear PDEs via infinite-dimensional Lie brackets

**[01547] Optimization in BV and Measure Spaces: Theory and Algorithms**

- [02974] Proximal methods for point source localisation
- [04816] Nonsmooth minimization in Banach spaces meets sparse dictionary learning
- [04270]  $L^q$ -quasinorm sparse optimal control problems with controls in BV functions
- [04282] Robust Optimal Experimental Design for Bayesian Inverse Problems
- [03634] Opial property in Wasserstein spaces and applications
- [03671] An Optimal Transport-based approach to Total-Variation regularization for the Diffusion MRI problem
- [04791] A minimization problem in the space of bounded deformations arising in visco-plastic fluid flows
- [03554] Solving Discrete Subproblems of a Trust-Region Algorithm for MIOCP
- [03555] Regularization and outer approximation for optimal control problems in BV
- [03256] On integer optimal control problems with total variation regularization
- [04006] Non-uniform Grid Refinement for the Combinatorial Integral Approximation

**[01605] Recent advances in computational methods for kinetic and hyperbolic equations**

- [03143] A Natural Model Reduction Framework for Kinetic Equations

**[01622] Mathematics for Prediction and Control of Complex Systems**

- [02251] Sequential data assimilation and data driven control
- [02790] Data-driven Reconstruction of Partially Observed Dynamical Systems
- [02800] Sensor selection by greedy method for linear dynamical systems
- [02804] Fast Linear-regression-based Sensor Selection and its Applications
- [02789] Identifying Coherent Structures within Turbulent Flows over Roughness Obstacles
- [02825] Quantifying Weather Controllability and Mitigatable Flood Damage Based on Ensemble Weather Forecast
- [02885] Ensemble sensitivity and its potential applications in weather control
- [02518] Chaos implies effective controllability of extreme weather
- [02814] Noise Calibration for the Stochastic Rotating Shallow Water Equations
- [03049] Machine learning-based estimation of state-dependent forecast uncertainty
- [03126] Observability of continuous-time Markov model and filter stability
- [03024] On random feature maps in prediction

**[01661] Recent Development on the Methods and Applications of Complex PDE systems**

- [04291] A learned conservative semi-Lagrangian finite volume scheme for transport simulations
- [03990] A new type of simplified inverse Lax-Wendroff boundary treatment for hyperbolic conservation laws
- [02713] Transmission Dynamics of Tuberculosis with Age-specific Disease Progression
- [02985] Extended-release Pre-Exposure Prophylaxis and Drug Resistant HIV
- [04493] A Level-Set Framework for Implicit Solvation
- [04909] Adaptive ANOVA and reduced basis methods to anisotropic stochastic PDEs
- [04915] Theoretical Principles of Enhancer-Promoter Communication in Gene Expression

**[01671] Financial Modeling**

- [05403] Insurance design for the loss of epidemic outbreaks involving the Cramer -Lundberg model
- [02749] Micro-foundations of some financial models with bubbles
- [02787] An Ito-Wentzell Formula for SDE Conditional Measure Flows
- [04500] A Generalized Cramér-Lundberg Model Driven by Mixed Poisson Processes

**[01672] High accuracy compact methods for partial differential equations**

- [05366] Spectral Element Method for Parabolic Problems with Corner Singularities

**[01681] Recent advances in numerical methods for partial differential equations**

- [03945] Geometrical degrees of freedom for high order Whitney forms
- [02919] Energy-preserving Mixed finite element methods for a ferrofluid flow model
- [03132] Immersed CR element methods for the elliptic and Stokes interface problems
- [02917] A fast Cartesian grid method for unbounded interface problems with non-homogeneous source terms

- [04905] Staggered DG methods for elliptic problems on general meshes
- [04160] Accelerated Gradient and Skew-Symmetric Splitting Methods for Monotone Operator Equations
- [03693] Solve electromagnetic interface problems on unfitted meshes
- [03714] Pressure-robust virtual element methods for the Stokes problem on polygonal meshes
- [05142] Arbitrary order DG-DGLM method for hyperbolic systems of multi-dimensional conservation laws
- [04537] Implementation and Application of Virtual Element Method in FEALPy
- [05586] Convergence of an AWG method for indefinite time-harmonic Maxwell equations
- [04955] High order stable generalized finite element method for interface problems

**[01718] On SDP relaxations of polynomial optimization**

- [01976] Tightness conditions of SDP relaxation for QCQPs with bipartite graph structure
- [02464] Equivalent Sufficient Conditions for Exact SDP Relaxation and the Saddle Point of Lagrangian Function of QCQP
- [02214] Approximation Hierarchies for Copositive Cone over Symmetric Cone
- [02008] An inexact projected gradient method with rounding and lifting for rank-one semidefinite relaxation of polynomial optimization

**[01768] Computer-assisted proofs in differential equations**

- [04529] Numerical verification methods for ODEs with conservative quantity
- [04834] Computer-assisted Existence Proofs for Navier-Stokes Equations on an Unbounded Strip with Obstacle
- [04194] Relative equilibria for the n-body problem
- [05267] Chaos in Mackey-Glass: computation of transverse homoclinic orbits
- [05182] Smooth imploding solutions for 3D compressible fluids
- [02910] Computer-assisted proofs of localized patterns in the planar Swift-Hohenberg equation
- [05035] Rigorous computation of Poincare maps
- [02908] Validation of Elliptic Invariant Tori in Hamiltonian Systems
- [03720] Validated Numerics for divergent series via the Borel Transform
- [04398] Characterising blenders via covering relations and cone conditions
- [03900] Validated integration of semilinear parabolic PDEs
- [05270] Validated dynamics in neural networks: towards chaos
- [05292] Global Dynamics and Blowup in Some Quadratic PDEs
- [05275] Worrisome Properties of Symbolic Representations of Deep Neural Network Controllers
- [05090] A rigorous integrator and global existence for higher-dimensional semilinear parabolic PDEs via semigroup theory

**[01800] Numerical methods for fluid-structure interaction and poroelasticity**

- [03958] Space-time domain decomposition approach for Stoke flow coupled with poroelasticity
- [04129] Two-field any-order finite element solvers for poroelasticity problems
- [04672] A mathematical framework for poro-visco-elastic models
- [04316] An energy stable second-order method for three-phase flows
- [04829] Cell-Based Numerical Approach to Evaluate CTC Binding Behavior in Microfluidic Device
- [02971] A Banach spaces-based fully-mixed formulation for the Navier-Stokes/Darcy coupled problem
- [03829] Numerical simulation of the time-fractional Navier-Stokes-Fokker-Planck (tfNSFP) equation

**[01834] Structure analysis and dynamics modelling in graphs and networks**

- [03989] Evolutionary Game Theory on Dynamic Networks
- [02059] An efficient adaptive degree-based heuristic algorithm for influence maximization in hypergraphs
- [04046] Identifying vital nodes through augmented random walks on higher-order networks
- [04449] Emergence of Cooperation Through Coevolving Time Scale in Spatial Prisoner's Dilemma
- [01988] information-opinion dynamics on social multilayer networks
- [04619] Characterizing Cycle Structure in Complex Networks
- [03130] Collaborative deep learning framework for network inference and dynamical prediction
- [05541] Multichannel game on structured populations

**[01858] Interplay among Manifold Learning, Stochastic Calculus, and Volatility Estimation**

- [02841] Convergence of Hessian estimator from random samples on a manifold
- [02848] Limit Theorems for the Positive Semidefinite Modification of Malliavin-Mancino Estimator for the Spot Volatility Process
- [04489] Convergence of Laplacian and its rate for submanifolds that are not necessarily smooth
- [02761] On excursions inside an excursion
- [0,1]. We analyze the maximum heights of these
- [02842] Diffusion Estimation with Fourier-Malliavin Method
- [02849] Statistical Analysis with Geodesics and Curvature in Data Space
- [02840] A Quantitative Central Limit Theorem arising from Time-Frequency Analysis
- [02846] Market Price-Volatility Simulator
- [02733] A graph discretized approximation of diffusions on Riemannian manifolds

**[01868] An introduction of “Journal of Machine Learning” for applied mathematicians**

- [02598] Embedding Principle: A Hierarchical Structure of Loss Landscape of Deep Neural Networks

- [02247] Perturbational Complexity and Reinforcement Learning in Reproducing Kernel Hilbert Space
- [02258] The Random Feature Method for Solving Partial Differential Equations
- [02957] DeePN<sup>2</sup>: A deep learning-based non-Newtonian hydrodynamic model
- [02982] Generalization ability and memorization phenomenon of distribution learning models
- [04035] Approximation of Functionals by Neural Network without Curse of Dimensionality
- [02256] Approximation of Functionals by Neural Network without Curse of Dimensionality
- [02998] Ab-Initio Study of Interacting Fermions at Finite Temperature with Neural Canonical Transformation
- [01897] New Tools for Nonlinear Time Series Analysis**
  - [05007] Pattern-based approaches to identifying coupling structures among multivariate time series
  - [03507] Transition network approaches for nonlinear time series analysis
  - [04058] Persistent homology induced by ordinal patterns for multivariate time series
  - [04580] Reconstruction of causal graphs with self loops
  - [03926] Power spectrum estimation for extreme events data
  - [04346] Constructing First Return Maps from Ordinal Partitioning of Time Series
  - [04581] Optimization approaches in analyzing marked point process data
  - [02926] Generalized entropies in nonlinear time series analysis
- [01933] Fluid-structure interactions in Stokes flows**
  - [04825] Cross-stream migration of vesicles in vortical flows
  - [04962] Confinement effects on a suspension of squirmers
  - [04477] Hydrodynamics and rheology of fluctuating, semiflexible, inextensible, and slender filaments in Stokes flow
  - [04813] Numerical simulations of swimming with multiple bacterial flagella
  - [05143] A multiscale framework for rigid bodies in Stokes flow with applications to nanocellulose
  - [04881] Bounds on particle configurations in an active suspension
  - [04858] Drag force on spherical particles trapped at a liquid interface
  - [05148] Bacterial collective motion and spread in porous media
  - [02866] Soft magnetic microrobots move more efficiently with a flat tire
  - [05297] Bacterial swarming above surfaces with friction
- [01935] Advances in Inverse Problems and Imaging**
  - [03733] Increasing stability in the linearized inverse Schrodinger potential problems
  - [03422] High-order boundary integral equation solvers for layered-medium scattering problems
  - [04333] An inverse boundary value problem for a nonlinear elastic wave equation
  - [04344] Inverse random scattering problems for stochastic wave equations
  - [04564] An Inverse Problem for Nonlinear Time-dependent Schrodinger Equations with Partial Data
  - [04099] Inverse scattering problems with incomplete data
  - [03745] Imaging of penetrable locally rough surfaces from phaseless total-field data
  - [04075] A new approach to an inverse source problem for the wave equation
  - [04288] Recovering an infinite rough surface by acoustic measurements
  - [03405] Uniqueness on recovering coefficients from localized Dirichlet-to-Neumann map for piecewise homogeneous piezoelectricity
- [01952] Mathematical models of morphogenesis and morphological deformation in living organisms**
  - [02830] A kinetic model for sol-gel transition of teleost muscular proteins
  - [03680] Mathematical model for dynamics of endothelial cells in sprouting angiogenesis
  - [04407] Measurement and mathematical analysis of organ morphogenetic processes
  - [03395] A mathematical model for the evolution of low-grade gliomas before and after radiotherapy
- [01996] Control and inverse problems on waves, oscillations and flows**
  - [03795] Recovery in vivo viscoelasticity from elastography measured data
  - [03880] Acousto-electric tomography imaging model and algorithm based on two-point gradient method
  - [04269] Numerical method for unique continuation of elliptic equations and applications
  - [04089] Reconstruction of piecewise smooth diffusion coefficient and initial value with adaptive regularization
  - [04229] Inverse problems for the Duffing equation in pediatrics
  - [04402] Unique determination of source and Robin coefficient in fractional diffusion equation
  - [05327] Fine-tuning neural-operator architectures for training and generalization
  - [03684] Reconstruction of location for a single point target in time-domain fluorescence diffuse optical tomography
  - [05416] STABILITY ESTIMATES FOR AN INVERSE PROBLEM FOR SCHRODINGER OPERATORS AT HIGH FREQUENCIES FROM ARBITRARY PARTIAL BOUNDARY MEASUREMENTS
  - [04623] Carleman estimates and some inverse problems for the coupled quantitative thermoacoustic equations
  - [02703] Numerical reconstruction of the spatially dependent source term in a time-fractional diffusion equation
  - [04572] Unique continuation for wave equations in asymptotically anti-de Sitter spaces
- [02012] Splitting Optimization: Theory, Methodology and Application**
  - [02878] Decentralized Entropic Optimal Transport for Privacy-preserving Distributed Distribution Comparison
  - [02881] An alternative extrapolation scheme of PDHGM for saddle point problem with nonlinear function
  - [02882] A balanced Douglas-Rachford splitting algorithm for convex minimization
  - [02904] A projection-like method for quasimonotone variational inequalities without Lipschitz continuity

- [02918] A trust-region-based splitting method for linear constrained programs
- [02995] A Decentralized Second-Order Multiplier Algorithm with Quasi-Newton Tracking
- [03066] Tight Convergence Rate in Subgradient Norm of the Proximal Point Algorithm
- [03073] A fast PIRNN algorithm for nonconvex low-rank matrix minimization problems
- [03085] Gradient methods using Householder transformation with application to hypergraph partitioning
- [03102] Solving saddle point problems: a landscape of primal-dual algorithm with larger stepsizes
- [03200] Inexact variable metric proximal incremental aggregated gradient algorithm for nonconvex nonsmooth optimization problem
- [03253] A Restricted Dual PRSM for a Strengthened DNN Relaxation for QAP

**[02014] High-order numerical methods: recent development and applications**

- [03002] High-order Structure-Preserving Schemes for Special Relativistic Hydrodynamics
- [03400] High order entropy stable and positivity-preserving discontinuous Galerkin method for the nonlocal electron heat transport model
- [02764] A new cut-cell interface treating method for compressible multi-medium flow
- [02690] A hybrid WENO scheme for steady Euler equations in curved geometries on Cartesian grids
- [03089] Error estimates to smooth solutions of high order Runge–Kutta discontinuous Galerkin method for scalar nonlinear conservation laws with and without sonic points
- [02994] Energy stable discontinuous Galerkin methods for compressible Navier–Stokes–Allen–Cahn System
- [02714] Superconvergence of LDG method for nonlinear convection-diffusion equations
- [03001] An essentially oscillation-free discontinuous Galerkin method for hyperbolic conservation laws
- [03431] Structure-preserving methods for Boltzmann continuous slowing down equations
- [03359] Positivity-preserving high-order DG method for weakly compressible two-phase flows
- [03039] On Entropy Conservative and Stable Discontinuous Galerkin Spectral Element Methods
- [03065] Affine-Invariant WENO Weights and their applications for hyperbolic conservation laws
- [03094] Arbitrary high-order fully-decoupled numerical schemes for phase-field models of two-phase incompressible flows
- [03096] Accuracy-enhancement of discontinuous Galerkin methods for PDEs containing high-order spatial derivatives
- [03105] A discontinuous Galerkin method for the Camassa–Holm–Kadomtsev–Petviashvili type equations
- [03349] High order finite difference WENO methods with unequal-sized sub-stencils for the DP type equations

**[02015] Theory and applications of random/non-autonomous dynamical systems part II**

- [03870] Worked out examples of Random Relaxed Newton's Methods
- [02705] Complex two-dimensional random relaxed Newton's methods
- [02999] New Q-Newton's method and Backtracking line search
- [05306] A Universal Fatou Component

**[02017] Recent progress in theory and applications of time-delay systems**

- [04818] Delay induced self-sustained oscillations in the Nonlinear Noisy Leaky Integrate and Fire model for networks of neurons.
- [04601] Global stability of multi-cell reaction systems with arbitrary time delays
- [04324] Time lag monotonicity-breaking in time-delay systems with impulses
- [03244] Mode Selection Rules for multi-Delay Systems
- [04187] Blow-up of solutions to some delay differential equations
- [03602] Absolute stability and absolute hyperbolicity in systems with time-delays
- [03557] Delay-dependent stability switches in delay differential systems
- [05023] Stabilization of periodic orbits with complex characteristic multipliers via DFC
- [03942] “Mild solutions” for hereditary linear differential systems
- [04145] Linearized instability for neutral functional differential equations with state-dependent delays
- [03765] Morse decomposition of the global attractor for delay differential equations

**[02023] Theory and applications of random/no-autonomous dynamical systems part IV**

- [05589] Physical applications of infinite ergodic theory
- [03122] Transition to Anomalous Dynamics in A Simple Random Map
- [05573] Arcsine law for random dynamics with a core
- [05570] Infinite ergodic theory in physics

**[02025] Recent Advances on the Analysis and Applications of Continuous and Discrete Integrable Systems**

- [03558] Integrable boundary conditions for quad-graph systems: classification and applications
- [03221] Geometric Aspects of Miura Transformations
- [04193] Curvature equation with conic singularities and integrable system
- [03194] A Generalization of an Integrability Theorem of Darboux and the Stable Configuration Condition.
- [03560] Rogue waves and their patterns in the vector nonlinear Schrödinger equation
- [03656] Whitham modulation theory of Riemann problem for nonlinear integrable equations
- [03369] Quantum variational principle for Lagrangian 1-forms
- [05098] Three-dimensional fundamental diagram of stochastic cellular automata
- [05088] Beyond the Painlevé property
- [05195] Constructing non-commutative systems with Pfaffian type solutions

[03957] Addition formulae for ultradiscrete hafnians

[05092] Recent Advances on the Analysis and Applications of Continuous and Discrete Integrable Systems

**[02056] Recent Advances in Partitioning Method for the Structures**

[03920] Displacement-only Partitioned Equations for Structures without Lagrange Multipliers

[04749] Displacement-based dynamic analysis of partitioned structural systems

[04659] Partitioned Damage Identification of Structural Systems

[03098] Development of partitioning method for thermoelastic Interaction Problems with energy flux constraint

[04222] A Componenet Mode Synthesis Method Using a Displacement-Based Partitioned Approach

[03460] Iterative Algorithm for Quasistatic Structural Problems Employing Only Partitioned Displacements

**[02060] Topics in extremal graph theory**

[02678] Spanning trees in sparse pseudorandom graphs

[03075] Extremal results on 4-cycles

[03224] Many Hamiltonian subsets in large graphs with given density

[03146] Balanced Subdivisions in Graphs

**[02067] Recent topics on generalized orthogonal polynomials and their applications**

[04542] Meta algebras, biorthogonal rational functions and the Askey scheme

[04588] Introducing  $q \rightarrow 1$  limits of biorthogonal rational functions: two instructive examples

[03379] CMV bispectrality of polynomials orthogonal on the unit circle

[04976] The Element Distinctness Problem Revisited

[02693] Christoffel Transformations for (Partial-)Skew-Orthogonal Polynomials and Applications

[02730] Multiple skew orthogonal polynomials and two-component Pfaff lattice

[04996] Another Type of Forward and Backward Shift Relations for Orthogonal Polynomials in the Askey Scheme

**[02072] Theory and applications of random/non-autonomous dynamical systems: Part I**

[03478] New characterizations of noise-induced order

[04094] Time-delayed feedback control for random dynamical systems

[03936] Rigorous enclosure of spectra and its applications

[03935] Recent developments on Lorenz-like attractors

**[02083] Integrable Aspects of Nonlinear Wave Equations, Solutions and Asymptotics**

[05581] Recent results on the Fractional Nonlinear Schroedinger Equation

[05588] Duality of positive and negative integrable hierarchies via relativistically invariant fields

[04900] Integrable Deep Learning--PINN based on Miura transformations and discovery of new localized wave solutions

[04206] Drinfeld-Sokolov hierarchies and diagram automorphisms of affine Kac-Moody algebras

[04907] On the long-time asymptotics of the modified Camassa-Holm equation in space-time solitonic regions

[05585] Local and global analyticity for a generalized Camassa-Holm system

[04390] Long-time asymptotics for the defocusing NLS equation with step-like boundary conditions

[05490] New revival phenomena for bidirectional dispersive hyperbolic equations

[05580] Darboux transformation and soliton solutions for a generalized Sasa-Satsuma equation

[05584] Rogue waves and solitons of nonlinear integrable/nearly integrable systems

[05579] The modified KdV equation on the background of elliptic function solutions

[04134] Pattern Transformation in Higher-Order Lumps of the Kadomtsev-Petviashvili I Equation

**[02109] Recent Advances on Numerical Analysis of Integral and Integro-differential Equations**

[02677] An hp-version of the discontinuous Galerkin method for fractional integro-differential equations with weakly singular kernels

[03691] Implicitly Linear Jacobi Spectral-Collocation Methods for Weakly Singular Volterra-Hammerstein Integral Equations

[03565] A collocation based approach for the numerical solution of singular fractional integro-differential equations

[02147] Solutions of second kind Fredholm integral equations by discrete projection methods

[03563] Numerical solution of fractional integro-differential equations

[04175] A new linearized maximum principle preserving and energy stability scheme for the space fractional Allen-Cahn equation

[03914] High accuracy analysis of FEMs for several time-fractional PDEs

[02240] Discontinuous piecewise polynomial collocation methods for integral-algebraic equations of Hessenberg type

[04726] Mean square exponential stability and practical mean square exponential stability of stochastic delay differential equations driven by G-Brownian motion and Euler-Maruyama approximations

[02676] Superconvergent postprocessing of the continuous and discontinuous Galerkin methods for nonlinear Volterra integro-differential equations

**[02115] Theory and applications of random/non-autonomous dynamical systems Part III**

[04171] Arcsine and Darling-Kac laws for piecewise linear random interval maps

[04000] Generalized uniform laws for occupation times of intermittent maps

[04085] Estimates of invariant measures for random maps

[04503] probability and ergodic theory for inner functions

**[02130] Fluid-structure interactions in geophysical flows**

- [04348] How Fluid-Mechanical Erosion Creates Anisotropic Porous Media
- [04569] Moving boundaries in thermal convection
- [04835] Using asymptotic analysis to improve numerical methods for multiphase flows
- [04665] Laser shot on water and ice
- [04383] A simple model on what drives continental drifts
- [05512] Computing the diffusivity of a particle subject to dry friction with colored noise
- [04815] The Formation of Karst Pinnacles

**[02154] Hypergeometric functions in statistics and particle physics**

- [03807] Towards Algebraic Analysis of Hypergeometric Systems
- [03843] D-Module Techniques for Solving Differential Equations in the Context of Feynman Integrals
- [04120] Distribution of eigenvalues of a singular elliptical Wishart matrix
- [04121] Restriction algorithms for holonomic systems and their applications
- [04146] Twisted cohomology and likelihood ideals
- [04152] Algebraic A-hypergeometric Laurent series and residues
- [04334] Sampling from toric models and hypergeometric functions

**[02163] Recent Developments in Stochastic Numerics and Computational Finance**

- [03032] Policy improvement algorithm for an optimal consumption and investment problem under general stochastic factor models
- [03381] Growth in Fund Models
- [03015] Carbon Emissions Pricing by Forward and Double Barrier Backward SDE approach
- [03307] Irreversible consumption habit under ambiguity: singular control and optimal G-stopping time
- [03674] New deep NN architecture using higher-order weak approximation
- [03488] A higher order discretization scheme for backward stochastic differential equations combined with a non-linear discrete Clark-Ocone formula
- [03622] New deep learning-based algorithms for high-dimensional Bermudan option pricing
- [05412] On-Policy and Off-Policy q-Learning in Continuous Time
- [03150] An Approximation Scheme for Path-Dependent BSDEs
- [03659] Practical high-order recombination algorithms for weak approximation of stochastic differential equations : Recursive patch dividing and its effects to singularities of terminal conditions
- [03645] Extended Milstein scheme for hypoelliptic diffusions
- [03489] Wong-Zakai approximation for stochastic PDEs and HJM model

**[02169] Recent advances on numerical methods for stochastic ordinary differential equations**

- [03230] Deterministic implicit two-step Milstein methods for stochastic differential equations
- [03158] Numerical methods for stochastic singular initial value problems
- [03262] A Positivity Preserving Lamperti Transformed Euler-Maruyama Method for Solving the Stochastic Lotka-Volterra Competition Model
- [03037] Convergence rate in  $L^p$  sense of tamed EM scheme for highly nonlinear neutral multiple-delay stochastic McKean-Vlasov equations

**[02178] Efficient computational methods for data matrices: exploiting sparsity and structure**

- [04733] Structured Matrices in Unsupervised Cross-Validation
- [04283] Randomized Algorithms for Rank Structured Matrices
- [03473] Scalable Data Analytics using Sparse Matrices
- [04632] Structure of Fisher information matrices in deep learning
- [04795] Exploiting Supernodal Structures in Sparse All Pair Shortest Path Computation.
- [04585] Optimizations of H-matirx-vector Multiplication for Many-core Processors
- [04849] Distributed Graph Neural Network for Billion-Scale Graphs
- [05081] A Framework to Exploit Data Sparsity in Tile Low-Rank Cholesky Factorization

**[02181] Numerical methods and analysis for linear systems and eigenvalue problems**

- [03254] Interpretation of partial convergence from space partition for linear systems
- [04340] The FEAST algorithm accelerated by subspace expansion for eigenproblems
- [03264] Computing eigenvalues of semi-infinite quasi-Toeplitz matrices
- [03454] Preconditioning techniques for nonlinear eigenvalue problem expressed in non-monomial basis
- [04543] A variant algorithm of the IDR(s) method for solving linear systems
- [03550] Randomized block Kaczmarz methods with k-means clustering for solving linear systems

**[02212] Modeling, Algorithms and Simulations for Flow and Transport in Porous Media**

- [03292] Stabilized enhancement for large time computation using exponential spectral process method
- [03294] A pressure robust solver for Stokes flow based on a lifting operator
- [03331] Numerical Approaches and Analysis for The Generalized Maxwell-Stefan Equations
- [03419] The Undrained Split Phase Field Method for Modeling Hydraulic Fracture Propagation
- [03443] Accelerating Pressure-Temperature Flash Calculations with Physics-informed Neural Networks
- [03499] The numerical CFD-DEM model for polymer flooding in weakly consolidated porous media
- [03503] Physics-Preserving Semi-Implicit Schemes for Porous Media Flow with Capillary Heterogeneity
- [04169] Efficient numerical methods for thermodynamically consistent model of two-phase flow in porous media

[05155] Geothermal management with an integrated optimization method accelerated by a general thermal decline model and deep learning

[05424] Gym-preCICE: Reinforcement Learning Environments for Active Flow Control

[05495] Ensemble schemes for the numerical solution of a random transient heat equation with uncertain inputs

**[02219] Pattern formation and propagation in reaction-diffusion systems on metric graphs**

[05005] Invasion analysis for population dynamics models on simple metric graphs

[02969] Propagation phenomena of Fisher-KPP equation in a shifting environment

[03115] Pulse dynamics for reaction-diffusion systems on various metric graphs

[03288] Reaction-advection-diffusion equations over simple graphs

[04149] The effect of advection on spike solutions for the Schnakenberg model on Y-shaped metric graph

[03837] Turing instability and bifurcation in reaction-diffusion systems on metric graphs

[04417] Front propagation for Lotka-Volterra competition-diffusion system on unbounded star graphs

**[02221] Recent progress on mathematical theory of boundary layer**

[03046] Eckhaus instability of the compressible Taylor vortex

[03064] Stability of shear flows in inviscid and viscous fluids

[03247] Tollmien-Schlichting waves in the subsonic regime

[04253] Global Existence of Weak Solutions for Compressible Navier-Stokes-Fourier Equations with the Truncated Virial Pressure Law

[03513] Nonlinear Stability of the Taylor-Couette flow

[04401] On the solvability of the linearized Triple-Deck system

[03016] On dynamic stability for steady Prandtl solutions

**[02277] New regularizing algorithms for solving inverse and ill-posed problems**

[05628] Regularization of linear inverse problems and neural networks

[05627] Applied inverse problems for parabolic equations

[02806] Data-Driven Regularization in Variational Data Assimilation from An Ocean Perspective

[02803] Uniqueness and numerical inversion in the time-domain fluorescence diffuse optical tomography

[02839] Stochastic asymptotical regularization for nonlinear ill-posed problems

[03062] A new framework to quantify the uncertainty in inverse problems

[03104] Numerical algorithms for solving the nonlinear Schrödinger equation

[03354] Multidimensional Ill-Posed Problems in Applications

[04375] Solution of inverse problems in three-dimensional singularly perturbed PDEs

[05101] The coupled complex boundary methods for inverse problems of partial differential equations

[05498] Physics-informed invertible neural network for the Koopman operator learning

**[02285] New Trends in Tensor Networks and Tensor Optimization**

[03267] Efficient Machine Learning with Tensor Networks

[05506] Accelerated Doubly Stochastic Gradient Descent for Tensor CP Decomposition

[03184] Tensor network strcuture search

[04779] Towards Multi-modes Outlier Robust Tensor Ring Decomposition

[05508] Singular Value Decomposition of Dual Matrices and its Application to Traveling Wave Identification in the Brain

[03043] Multilinear Pseudo-PageRank for Hypergraph Partitioning

[04276] Tensorial Time Series Prediction via Tensor Neural Differential Equations

[03838] A gradient projection method for semi-supervised hypergraph clustering problems

**[02327] Stability of Numerical Linear Algebra Algorithms**

[02923] A projection method for singular eigenvalue problems of linear matrix pencils

[03257] Backward stability in rational eigenvalue problems solved via linearization

[03008] Computing the matrix sign function with the double exponential formula

[03899] Mixed Precision Strategies for Preconditioned Restarted GMRES

[04236] Numerical stability of block classical Gram-Schmidt process

[02742] Cross-interactive residual smoothing for block Lanczos-type methods for solving linear systems with multiple right-hand sides

[02706] Gauss-Seidel (MGS) - Jacobi (CGS) GMRES with Rank-1 Perturbation Smoothers

[05049] Improving convergence and stability of Krylov subspace methods for solving linear systems

**[02342] On dataset sparsification and data reconstruction in deep learning**

[03191] Data sampling for surrogate modeling and optimization

[03317] Bayesian inference via dataset sparsification

[03934] Foundations of Information Leakage in Machine Learning

[04492] Understanding Reconstruction Attacks with Dataset Distillation

**[02349] Deep Implicit and Explicit Models for Inverse Problems: Hybrid Data-Driven Models, Neural ODEs, PDEs and Beyond**

[05633] Why Deep Surgical Models Fail?: Revisiting Surgical Action Triplet Recognition through the Lens of Robustness

[05634] On Implicit Neural Representation

- [03463] Learning pair-wise homeomorphic image registration in a conformal-invariant hyperelastic setting
- [03252] Spherical Image Inpainting with Frame Transformation and Data-driven Prior Deep Networks
- [05441] Learning to solve inverse problems with unsupervised nonlinear models
- [04181] A learning framework for mapping problems via Quasiconformal geometry
- [05328] Physics Informed Graph Transformer for PDEs
- [03627] Continuous U-Net: Faster, Greater and Noiseless

**[02370] Recent advances in Ultrasound Biomedical Imaging**

- [05140] Applications of Spatial Coherence to Ultrasonic Imaging
- [04772] A local space-invariant approximation for DAS Point Spread Function computation
- [03464] Design and 3-D medical applications of 2-D ultrasound sparse arrays
- [04653] Recent advances in array and sequence design for 3D and high frame rate medical ultrasound imaging

**[02376] Recent Advances in Dynamic Games and Control Theory and Their Connection to Data Science**

- [03672] The Role of Information Structure in Games and Learning
- [02854] Optimal transaction mechanism for dynamic storage management game in smart grid
- [02858] Reinforcement Learning Algorithm for Mixed Mean Field Control Games
- [02930] Recent Advances on Fractional Optimal Control Problems
- [03245] Stabilizability of Nash equilibrium
- [04475] Cooperation and Cost Sharing Problems in Supply Networks
- [03268] Hodge allocation for cooperative rewards

**[02386] Recent advances on theory and algorithms in deep learning applications**

- [03440] Vanilla Feedforward Neural Networks as a Discretization of Dynamical Systems
- [03441] Phase Diagram of Initial Condensation for Two-layer Neural Networks
- [03386] Robust Full Waveform Inversion: A Source Wavelet Manipulation Perspective
- [02945] Learning robust imaging model with unpaired data
- [03329] Generative Models Based Statistical Priors for Compressive Sensing and Medical Imaging
- [03483] Normalizing-flows based design of experiments for failure probability estimation
- [03477] Unsupervised learning driven by Langevin dynamics and its applications to inverse problems
- [03450] Self-supervised Deep learning Methods in Imaging

**[02387] Recent Advances on Distributed Optimization**

- [03522] Optimal Gradient Tracking for Decentralized Optimization
- [03541] Optimal Complexity in Distributed Learning with Communication Compression
- [03556] Asymptotic Network Independence in Distributed Stochastic Gradient Methods
- [03570] Unified and Refined Analysis of Decentralized Optimization and Learning Algorithms

**[02392] Low-Rank Models in Data Science**

- [02769] Low-rank models in data science: Applications and optimization challenges
- [05455] Low Rank Matrix Recovery from Column-wise Projections: Fast and Communication-Efficient Solutions
- [04491] Tensor-Norm Approaches to Low-Rank Matrix Recovery by Convex Program
- [04277] Algorithmic approaches to recovering sparse and low-rank matrices
- [03939] Bures-Wasserstein Methods in Matrix Recovery
- [05442] Improved Global Guarantees for Low-Rank Models via Rank Overparameterization
- [04377] Tensor Completion via Tensor Train Based Low-Rank Quotient Geometry under a Preconditioned Metric
- [04975] Iteratively Reweighted Least Squares for Low-Rank Optimization: Optimality & Convergence Rates
- [04701] Multi-window Gabor phase retrieval

**[02396] Recent Advances on Polynomial System Solving**

- [03796] Polynomial System Solving in a Nutshell
- [04394] Signature-based algorithm and change of ordering for Groebner basis
- [03913] Dimension results for polynomial systems over complete toric varieties
- [03633] On the computation of staggered linear bases
- [03688] Square-Free Pure Triangular Decomposition of Zero-Dimensional Polynomial Systems
- [05286] On the bit complexity of roadmap algorithms
- [03750] Solving semi-algebraic systems arising in applications
- [04993] Root Separation Bounds

**[02402] Numerical methods for a class of time-dependent PDEs**

- [02681] Unconditionally MBP-preserving linear schemes for conservative Allen-Cahn equations
- [02717] Uniformly accurate nested Picard iterative integrators for the Klein-Gordon-Schrödinger equation in the nonrelativistic regime
- [02550] Structure-preserving scheme for the PNP equations
- [02553] Numerical simulation of rotational nonlinear Schrödinger equations with attractive interactions
- [02622] IMPROVED UNIFORM ERROR BOUNDS OF THE TIME-SPLITTING HERMITE SPECTRAL METHODS FOR THE LONG-TIME GROSS PITAEVSKII EQUATION WITH WEAK NONLINEARITY

**[02404] New Trends in Hierarchical Variational Inequalities and Optimization Problems**

- [03031] Self-adaptive subgradient extragradient method with extrapolation procedure for MSVIs
- [03050] Subgradient-extragradient method for SEP, VIP and FPP of multi-valued mapping

- [03061] Modified subgradient-extragradient method for monotone-bilevel-equilibria with VIP and CFPP constraints
- [03072] New strong convergence theorems of generalized quasi-contractive mappings
- [03144] Mittag-leffler stability of Fractional-order Neural Networks with time-varying delays
- [03170] Singular Riemann problems and their applications
- [03270] Gas-liquid Phase Transition Problem for Non-isentropic Compressible Euler Equations
- [03286] Accelerated subgradient-extragradient methods for VIPs and CFPPs implicating countable nonexpansive-operators
- [03591] The Behaviors of Rupture Solutions for a Class of Elliptic MEMS Equations

**[02406] European Research Council (ERC) information session**

- [03125] European Research Council (ERC): insight into funding opportunities
- [05538] Building a new mathematical adventure with ERC support.
- [05548] Extreme-scale Mathematically-based Computational Chemistry Synergy project
- [05567] A dedicated Project Development Office for Mathematics

**[02408] Recent advances in two-phase flow influenced by thermal fluctuations**

- [03080] The stochastic Navier-Stokes-Allen-Cahn system with singular potential
- [03081] On some stochastic phase-field models of Cahn-Hilliard-Cook type with logarithmic potential
- [03044] Temperature Effects in Generalized Diffusions
- [04783] Asymptotics of the stochastic Cahn-Hilliard equation with space-time white noise
- [03980] Weak error analysis for the stochastic Allen-Cahn equation
- [03932] On a convergent SAV scheme for stochastic phase-field equations
- [03355] Martingale solutions to the stochastic thin-film equation in two dimensions
- [04416] SOLUTIONS TO THE STOCHASTIC THIN-FILM EQUATION FOR INITIAL VALUES WITH NON-FULL SUPPORT
- [04240] Existence of positive solutions to stochastic thin-film equations in the case of weak slippage
- [04442] On finite speed of propagation for stochastic thin-film equations

**[02411] Recent Advances in Numerical Methods for Nonlinear Equations and Applications**

- [03387] Efficient iterative scheme for system of nonlinear equations
- [03084] Non-Linear GAC Model for GIS Image Segmentation of Deforestation in Nusajaya Malaysia
- [03352] Analysis of Love-type wave in a nonlocal piezoelectric composite
- [03396] Mathematical modelling of Wave Equation in Elastodynamics Problems
- [03928] Iterative Newton type methods with fractional derivatives
- [03702] A Hybrid Genetic Algorithm for Solving Nonlinear Systems and Applications
- [03357] Iterative Method for Efficiently Computing Generalized Inverses of Matrices
- [03376] Globally convergent iterative method for evaluating matrix sign function
- [03040] An Iterative scheme for finding simultaneous roots of nonlinear systems
- [03925] High-order iterative methods for solving nonlinear systems

**[02423] Non-standard finite element methods**

- [04214] A posteriori error estimation for a C1-virtual element method of Kirchhoff plates
- [03654] Stabilization-Free Virtual Element Methods
- [03806] Discontinuous Galerkin methods for magnetic advection-diffusion problems
- [03492] Some finite element divdiv complexes in three dimensions
- [04728] Adaptive FEM for Helmholtz equation with large wave number
- [03581] Stable Finite Element Scheme for Dynamic Ginzburg-Landau Equations
- [03508] Local bounded commuting projection operators for discrete finite element complexes
- [04168] The weak Galerkin method for elliptic eigenvalue problems

**[02426] Mathematics of turbulent transport and coherent structures**

- [04104] Analysis of transport by coherent structures; overview
- [04490] Analysis, modeling, and simulation of slow-fast quasilinear dynamical systems
- [04122] Steady coherent states in Rayleigh-Bénard convection
- [04022] Optimal heat transport using branching flows
- [04552] Optimisation of horizontal periodicity in steady Rayleigh-Bénard convection
- [04406] Chaos and unstable periodic orbits in subcritical Taylor-Couette flow
- [03988] The state-space structure of wall turbulence at high Reynolds numbers: a reduced-order model perspective
- [03140] Coherent structures and the direct cascade in two-dimensional turbulence

**[02435] Scaling Limits of Interacting Particle Systems**

- [05450] Ergodic properties of rank-based diffusions
- [04342] Systems with Riesz Interactions in the Mean-Field Regime
- [03026] Large Deviations for Multiscale Weakly Interacting Diffusions
- [05239] Hydrodynamic Limits of non-Markovian Interacting Particle Systems on Sparse Graphs
- [04551] Wave propagation for reaction-diffusion equations on infinite trees
- [03975] From the KPZ equation to the directed landscape
- [05115] Longtime behaviour of the stochastic FKPP equation conditioned on non-fixation
- [03336] The interacting multiplicative coalescent and Levy-like random fields

- [03511] Graphon mean field systems
- [03358] Strong convergence of propagation of chaos for McKean-Vlasov SDEs with singular interactions
- [03721] Nonlocal approximation of nonlinear diffusion equations
- [04156] Entropy-dissipation Informed Neural Network for McKean-Vlasov Type PDEs

**[02438] Recent advances in numerical multiscale methods**

- [03763] Super-Localized Generalized Finite Element Method
- [03861] An efficient multiscale approach for simulating Bose-Einstein condensates
- [04037] Multigrid/multiscale solver for the radiative transfer equation in heterogeneous media
- [03533] EXPONENTIALLY CONVERGENT MULTISCALE METHODS FOR HIGH FREQUENCY HETEROGENEOUS HELMHOLTZ EQUATIONS
- [03853] A high-order method for elliptic multiscale problems
- [04038] Hierarchical Attention Neural Operator for Multiscale PDEs
- [04167] An abstract framework for multiscale spectral generalized FEMs
- [03857] Multiscale multicontinuum problems in fractured porous media: dimension reduction and decoupling

**[02440] Advances in Optimization I**

- [04074] Some Recent Developments on Solving Variational Inequality Problems
- [05227] Monotone Variational Inequality (VI) for estimation and learning
- [04577] Implementation of Interior Point Method for Nonlinear Programming for Real-life Applications.
- [04650] Tropical convexity: application to linear programming and mean-payoff games
- [04479] Breaking the quadratic gap for strongly polynomial solvers to combinatorial linear programs
- [03172] Computational challenges in Flag Algebra proofs
- [03673] Improving Lower Bounds for Large Scale QAPs
- [03941] Closing Nonzero Duality Gaps in SDPs through Perturbations
- [04092] Maximum-Entropy Sampling: Algorithms and Application
- [03117] A role of semidefinite relaxation in mathematics of phase retrieval
- [03176] Exact Convergence Rate of Alternating Projections
- [05522] Bridging Distributional and Risk-sensitive Reinforcement Learning with Provable Regret Bounds

**[02445] Advances in Optimization II**

- [05543] Optimal Diagonal Preconditioning: Theory and Practice
- [03259] Smart Initial Basis Selection for Linear Programs
- [04683] Interior Point Methods are Not Worse Than Simplex
- [03175] Analysis of Algorithms on Growing Networks
- [03367] Two constructive techniques for producing linear extended formulations
- [03641] Interior-point methods on manifolds: theory and applications
- [03069] Alternating Linear Minimization: Revisiting von Neumann's alternating projections
- [03052] Combinatorial and geometric aspects of linear optimization
- [05126] On Some Optimization-Related Issues In Deep Learning
- [03071] Creating Collaborative Data Representations Using Matrix Manifold Optimization
- [03047] Accelerated and Sparse Algorithms for Approximate Personalized PageRank
- [04893] Optimal Composition Ordering for Linear Functions

**[02447] Advances in Diesel Engine Design and Control for Industry 4.0**

- [03642] XAI Based Fault Diagnosis for Steel Plates Manufacturing
- [04142] Distinguishability of linear control systems
- [04661] Optimizing Flow Parameters in Convergent Diesel Nozzles with Rough Walls
- [04696] In-Cylinder Combustion Investigation Against Some Injection Characteristics
- [04704] An Intelligent Control System for a Diesel Engine I
- [04750] In-Cylinder Combustion Investigation Against Some Injection Characteristics
- [04780] In-Cylinder Combustion Investigation Against Some Injection Characteristics
- [04965] Intake Plenum Design Improvement for a 12-Cylinder Diesel Engine
- [05053] Numerical Investigation of HCCI Combustion in the High Pressure Engine

**[02448] Verified Numerical Computations and Applications**

- [02902] High relative accuracy computing with the Cauchon algorithm
- [03658] Floating-point matrices with specified solutions for linear algebra problems
- [05571] Adaptive precision sparse matrix-product and application to Krylov solvers
- [05577] Iterative refinement for an eigenpair subset of real symmetric matrices
- [05276] Lower Bounds for Smallest Singular-Values of Asymptotic Diagonal Dominant Matrices
- [05029] Error estimation for the FEM solution with a few bad elements
- [03173] Verified Numerical Computations for multiple solutions of the Henon equation
- [05290] Rigorous solution-enclosures of elliptic boundary value problems between piecewise linear functions
- [04361] Verified computation for shape derivative of the Laplacian eigenvalues
- [04568] Constructive error estimates for a full-discretized periodic solution of heat equation
- [03685] A Numerical verification method for a self-similar solution to the linear elliptic differential equation

[04321] A computer-assisted proof for a nonlinear differential equation involved with self-similar blowup in wave equations

**[02458] Progress and Challenges in Extreme Scale Computing and Big Data**

- [05261] Toward Post-Exascale Software-Ecosystem Sustainment
- [03388] Task-based hybrid parallel matrix factorization for distributed memory environment
- [03651] Accelerating lattice Boltzmann method with GPU and C++ standard parallelization
- [05041] GPU-accelerated viscoelastic crustal deformation analysis with data-driven method
- [03035] System-Wide Coupling Communication for Heterogeneous Computing Systems
- [03261] h3-Open-UTIL/MP: a coupling library for heterogeneous computing
- [03652] Modernizing the weather prediction model ICON for extreme-scale computing, a librarization effort
- [03776] Performance Modeling Challenges in Extreme Scale Computing
- [05260] Exascale challenges and opportunities for fundamental research
- [03605] An algorithm reducing by 2 the number of operations for the PageRank method, and its generalisation for stochastic matrix-vector products
- [03705] Accelerating Cardiac Electrophysiology Simulations using novel AI Hardware
- [05304] A Medical Data Analytics Framework Transforming Big Data to Better Healthcare

**[02470] Chaotic Supremacy Revolution**

- [03810] Chaos-like behavior of two-dimensional optical bistable device with external feedback
- [03967] Quantification of Orbital Instability of Chaotic Laser Diodes by Modified Orbital Expansion Exponent
- [03992] Development of MLD-TDS applying spintronic THz emitters excited by laser chaos light
- [04023] Application of entropic chaos degree to Lorenz system
- [04036] Stable THz waves using laser chaos
- [04083] Quantum walk analysis of spatial distribution of dressed-photon-phonon
- [04616] Quantum Fields as Category Algebras
- [05241] Exactly Solvable Chaos and Its Use to Realize Chaotic Supremacy

**[02474] Applied and Computational Dynamics**

- [03364] Connectedness of graphs of dynamical systems
- [03770] Changes in basin of attraction by homoclinic and heteroclinic tangencies in passive dynamic walking
- [04997] A novel bifurcation in hybrid dynamical systems: a model of human locomotion and its generalization
- [03723] Coupled Hopf bifurcations: interaction between Fitzhugh-Nagumo neurons
- [04209] A method of computing Morse decomposition via approximate ODE solvers and its application
- [03407] Finite-resolution recurrence in dynamical models
- [04891] Reconstruction of stationary measures from 'cycles' in random dynamical systems
- [03823] Computer verifiable criteria for chaos in piecewise smooth dynamical systems

**[02479] Recent advances for modeling, numerical algorithm, and applications in electronic structure calculation**

- [04686] Numerical method for the Elasticity Transmission Eigenvalues
- [03287] A multi-mesh adaptive finite element method for Kohn-Sham equation
- [03432] Mathematical theory and numerical methods for Bose-Einstein condensation with higher order interactions
- [03403] Solving Schrodinger equation using tensor neural network
- [04589] Computations of the ground states and collective excitations of Bose-Einstein condensates
- [03384] Multilevel correction adaptive finite element method for Kohn-Sham equation
- [03227] The Wigner function of ground state and one-dimensional numerics

**[02491] Mathematics of Epidemics: modelling, data analysis, and control**

- [03453] Optimal vaccination at high reproductive numbers: sharp transitions and counter-intuitive allocations
- [04794] An epidemic model for reinfection dynamics with heterogeneous susceptibility
- [03972] Effective screening with rapid antigen tests for COVID-19 patients: simulation with viral dynamics model
- [03510] Evaluation of Effectiveness of Global COVID-19 Vaccination Campaign in 2021
- [03458] Exploring the dynamics of contagion models with stages
- [04574] Mathematical modeling of COVID-19 transmission with pandemic response in South Korea
- [03885] Front propagation in an epidemiological model with mutations
- [05100] Resolving the enigma of COVID-19 outbreaks in Iquitos and Manaus

**[02493] Advanced Modelling of Complex Nonlinear Systems**

- [03289] A Minimal Set of Koopman Eigenfunctions -- Analysis and Numerics
- [03525] Acoustic Streaming
- [04735] The Underlying Correlated Dynamics in Neural Training
- [05114] A Nonstochastic Control Approach to Optimization

**[02499] Machine Learning for dynamics and its applications**

- [04040] Construction of differential equations from scalar chaotic time series
- [04709] Data-driven inference of Navier-Stokes turbulence from limited observations
- [03862] Long-lead prediction of Indian Summer Monsoon onset with reservoir computing
- [03000] Learning Strange Attractors with Reservoir Systems
- [04147] Dynamical system properties of reservoir computing models
- [02889] Predicting tipping point with machine learning

- [02921] Machine Learning for Predicting Missing Dynamics
- [05374] Kernel Flows and Kernel Mode Decomposition for Learning Dynamical Systems from Data
- [05420] Discovery of quasiperiodically driven dynamics using kernel methods
- [05427] Reservoir Computing Generalized
- [05429] Reservoir computing with the Kuramoto model
- [05431] Embedding bifurcation structures into a soft robotic actuator
- [05402] Physical reservoir computing using dynamics of biological neuronal network with modular structure

**[02514] Developing Performance Portable, Scalable and AI enabled Fusion Energy Physics Framework**

- [04465] Develop next generation CFD tools using AI libraries
- [04466] Cheap training sets of gyrokinetic surrogate models with active learning
- [04627] Implementation of a finite element PDE solver in AMReX
- [04652] AI deconvolution operator for plasma turbulent simulations on complex geometries
- [04741] Performance and scaling of amrPX: a multiphase CFD framework
- [05229] A highly parallel simulation of patient-specific hepatic flows

**[02515] Novel deep learning methodologies in Industrial and Applied Mathematics**

- [05353] Artificial Intelligence for Wind Turbine Predictive Maintenance
- [03575] Innovative Models for Explainable Artificial Intelligence
- [05376] Applications of Quaternion Monogenic Signal ConvNet Layer
- [05352] Novel deep learning methodologies in Industrial and Applied Mathematics
- [05354] AI Lifecycle Zero-touch Orchestration within the Edge-to-Cloud Continuum for Industry 5.0

**[02526] Recent Developments of Mathematical Economics Focusing on Macroeconomic Dynamics**

- [04358] On growth cycles in a stochastic post-Keynesian model
- [03425] A Three-Country Kaldorian Business Cycle Model with Fixed Exchange Rates
- [04424] Simple Estimations of the Natural Rate of Interest
- [04486] Dynamic Adjustment in the Mundell-Fleming Model

**[02527] AI for Healthcare and Medicine**

- [02894] Data Collaboration Cox Proportional Hazards Model for Privacy-preserving Survival Analysis
- [05307] AI-Enhanced Medical Imaging Analysis: Advancing Precision Treatment for NSCLC Brain Metastases
- [05001] Explainability and Fairness of Distributed Data Analysis
- [05362] Mitigating Non-IID Data Challenges in Federated Learning for Healthcare Applications
- [03888] Causal inference and machine learning on distributed data
- [05313] Precision Preventive Medicine in Sub-Healthy Population
- [03660] Medical AI, Biosensors and Privacy
- [05312] HeortaNet: AI for Quantifying Heart Structures on Non-Contrast CT Images

**[02533] Reliable and Efficient Numerical Computation of Nonlocal Models**

- [03174] The Effect of Domain Truncation for Nonlocal Models and Asymptotically Compatible Schemes in Numerical Computation
- [03775] Global well-posedness of one new class of initial-boundary value problem on incompressible Navier-Stokes equations and the related models
- [04201] High performance implementation of 3D FEM for nonlocal Poisson problem
- [03599] Asymptotical compatibility of a class of numerical schemes for a nonlocal traffic flow model

**[02537] Structured Low-Rank Matrices and Their Applications**

- [05519] Hierarchical Lowrank Arithmetic with Binary Compression
- [05545] Parallel Factorization of Hierarchical Matrices
- [05552] Parallel Low-Rank Approximation of High-Dimensional Multivariate Normal Probabilities on Manycore Systems
- [05590] A geometry oblivious H-matrix approximation scheme for rectangular matrices
- [05551] Dynamic Rupture Simulation Using FDP Method Accelerated by Lattice H-matrices

**[02541] Biochemical reaction network reduction methods & multiple timescale dynamics**

- [04793] The relationship between deterministic and stochastic quasi-steady-state
- [04404] Noise attenuation and ultrasensitivity in biological oscillators utilizing the multiple transcriptional repression mechanism
- [04800] Reduction of Chemical Reaction Networks with Approximate Conservation Laws
- [04454] A deep dive into the quasi-steady-state approximation to the Michaelis-Menten system
- [04203] Multiple timescales in reaction networks and the parametrisation method

**[02545] Challenges and Recent Advances in Phylogenetics**

- [04132] Navigating the Frontiers of Phylogenetic Research: Challenges and Applications
- [05050] Advances and challenges in statistical inference of phylogenetic networks
- [03613] The Tree of Blobs of a Species Network: Identifiability
- [03991] Identifiability of phylogenetic networks
- [04778] Log-concave density estimation on tree space
- [03260] Tropical Logistic Regression Model on Space of Phylogenetic Trees
- [04319] From phylogenetics to semigroups, through set partitions

- [04284] Learning from phylogenies to uncover evolutionary dynamics
- [05365] Minimum Number of Leaf-Covering Subtrees Covering Phylogenetic Networks
- [04243] Proximity measures for phylogenetic network classes
- [03534] Data reduction rules to compute distances between phylogenetic trees
- [03576] Parsimony and the rank of phylogenetic flattenings
- [04303] Phylogenetic X-cactuses
- [05034] On the Sackin index of galled trees
- [04250] Distribution of patterns in ranked tree-child networks
- [04323] Counting phylogenetic networks with the component graph method
- [02557] Collaboration of machine learning and physics-based simulation on earthquake disasters**
  - [04544] Physics-based long-period ground motion simulation for megaquakes
  - [03695] A smoothing scheme for seismic wave propagation simulation with SDWave
  - [04162] A quarter century of data from K-NET and KiK-net
  - [05004] Construction of strong motion database for data-driven ground-motion prediction models
  - [03553] Optimal Transport in Seismic Wave Analysis
  - [03984] Position-dependent inpainting for ground motion interpolation
  - [04967] Linkage of physics simulation and machine learning towards seismic risk assessment
  - [03740] Automated Building Damage Assessment using Multi-scale Siamese Deep Learning Network
- [02561] Mathematical Puzzles and Games in Theoretical Computer Science**
  - [04517] Uniqueness in puzzles and puzzle solving
  - [04855] The Complexity of Games and Puzzles with Limited Width
  - [04898] Mathematical Puzzles for Computer Scientists: Leisure or More?
  - [05028] One Cycle to Rule Them All
  - [05095] Generalized Jankens
  - [05219] Tilings and unfoldings
  - [05433] A Hardness Framework for Games and Puzzles: Motion Planning through Gadgets
  - [05443] Map Folding
- [02562] Recent development in data-driven modeling, data assimilation, and applications: meteorology, oceanography ionosphere, hydrology, environment**
  - [04677] Adaptive mesh atmospheric model development
  - [05293] A fast, high resolution pluvial flood model for risk assessment and real-time flood prediction
  - [04758] Data driven modelling and EnKF for spatial-temporal forecasting: Ozone and PM forecasting in China
  - [05285] Machine learning for data assimilation and predictability to the atmospheric models
  - [05103] Prediction of Swirling Fluid Flow Pattern in a River
- [02567] Data-driven Computational Mechanics for Structures, Structural Dynamics, and Materials**
  - [03299] Investigation on the hyper-reduction approach for the contact-impact simulation
  - [03428] Machine learning-based methods for the nonlinear structural analysis
  - [05003] Manifold-Augmented Deep learning-based Approach for Prediction of Airfoil Aerodynamic Performance at Low Reynolds Number
  - [03424] Model Order Reduction for Fluid-Structure Interaction Analysis via the Data-driven Machine Learning
  - [05031] Data-driven Model Reduction Approach for Multiscale Homogenization of Microstructure
  - [05220] An efficient neural network approximation of entropy solutions
  - [04471] Hypernetwork-based low-rank neural ordinary differential equations for solving parameterized partial differential equations
  - [05436] High-dimensional regression using partition of unity networks (POU-Net)
  - [05408] An augmented Lagrangian method to accelerate constrained optimization using hyperreduction
- [02569] Quantification of Business Uncertainties through Industrial Mathematics**
  - [03389] Mathematics behind performance estimation of multiscale structures
  - [04204] Handling Uncertainties in Decision Making
  - [04896] Aggregation value regression and its application to household demand forecasting
  - [04885] Ensemble based approaches for business uncertainty quantification
  - [04526] Topological methods for detection of uncertainties in Artificial Intelligence
  - [04919] Consecutive eigenvalues distribution of asymmetric quantum Rabi models
  - [05125] Changing the Misconception of Subsea Cable Laying Norm
  - [04095] Handling Uncertainties for Wastewater Treatment in Oxidation Pond
- [02570] Parameter Estimation, Targeted Observation, and Data Assimilation in Coupled Systems**
  - [04638] Improving Numerical Forecast Skill: Combinational Parameter Optimization and Coupled Data Assimilation
  - [05388] Application of the CNOP-PEP method in hydrological ensemble prediction in China to reduce model parameter uncertainties
  - [05401] The effect of Westerly Wind Burst on ENSO
  - [04422] Improving Model Uncertainty in Physical Parameterizations: Combinational Optimizations Using Genetic Algorithm in the Coupled Atmosphere-Chemistry Model
  - [03616] A novel approach of data assimilation: application to ENSO diversity predictions

- [04195] Exploring data-driven sparse sensor placement for determining rain gauge locations
- [04176] The Conditional Nonlinear Optimal Perturbation method and its application to the targeting observation for tropical cyclones
- [04998] Towards targeted observations of meteorological state for improving PM2.5 forecasts
- [03679] A case study of a dust event using the RAMS-MLEF atmosphere-aerosol coupled data assimilation system
- [04249] Impact of Soil Moisture Observation in the Coupled Atmosphere-Land Data Assimilation System
- [04599] Application and improvement of Land Data Assimilation System at CWB

**[02578] Interfaces and Mixing – Conservation Laws and Boundary Value Problems**

- [03293] Interaction between a particle and a liquid surface
- [03383] Smooth Navier-Stokes Solutions
- [03416] Determining control parameters for unsteady pulling of mass-spectrometry emitters
- [03716] Front Tracking Simulations of reshocked Richtmyer-Meshkov Instability
- [03735] Can environmental and intrinsic mechanisms of quantum mixing be distinguished experimentally?
- [03969] Exact solutions to nonlinear difference equations associated with Henon maps
- [03994] Nonlinear interaction of two nonuniform vortex interfaces and large vorticity amplification
- [04164] Compressible Kelvin-Helmholtz and Rayleigh-Taylor Instabilities
- [04478] Compressible Vortex Sheets and Free Boundary Problems
- [04545] Special self-similar class in Rayleigh-Taylor interfacial mixing
- [04546] Interface dynamics in ideal and realistic fluids
- [05008] Generalized Ideal Momentum Jet Model for Non-Circular Nozzle Geometries in Turbulent Pressure-Atomized Liquid Jets: Theoretical and Experimental Comparison
- [05070] A novel data analysis method for Rayleigh-Taylor mixing

**[02591] Recent advances in data-driven modeling and computational methods**

- [02896] Topological Data Analysis Experience in Malaysia: A Survey
- [03038] A Reaction Network Analysis of Insulin Signaling
- [03583] Comparing Lagrangian Particle Dispersion Models in Turbulent Flows: A Data-Driven Approach
- [03912] Error estimates of numerical methods for the Dirac equation
- [04021] A learning-based projection method for model order reduction of transport problems
- [04197] An iterative algorithm for POD basis adaptation
- [04384] Heat on hypergraph and its application to network analysis
- [04987] Convergence Rate Analysis for Deep Ritz Method

**[02600] Applied and computational discrete algorithms**

- [04306] Parallel Batch-Dynamic Graph Algorithms
- [03109] Approximation: a Paradigm for Designing Parallel Graph Algorithms
- [02991] Nested dissection ordering on GPUs
- [05454] Accelerating AI using Fast and Feasible Matrix Multiplication
- [03099] On heuristics for the Birkhoff-von Neumann decomposition
- [03435] Recent Advances in Streaming (Hyper)Graph Partitioning
- [04746] Efficient Data Structures for Sparse Dynamic Graphs
- [04669] Communication Efficient Stratified SGD on Distributed-Memory Systems

**[02612] Mathematical modeling of biofilm systems and applications**

- [03848] Simulation of ultrasonic biofilm detachment in membrane aerated bioreactors
- [04151] Bacterial Biofilms across scales and applications
- [04177] Microbially-influenced transport in sea ice
- [04844] Computational simulations of biofouling on ship hulls
- [05492] Long time behaviour of a thin-film model for early biofilm development

**[02613] Advances in Variational and Hemivariational Inequalities: Modeling, Analysis, and Applications**

- [04082] Recent Advances on Partial Differential Variational Inequalities
- [03283] Optimal control for variational inequalities of obstacle type
- [03248] Approximation techniques for solving hemivariational inequalities arising from contact mechanics
- [03265] A virtual element method for a quasistatic frictional contact problem
- [04032] The interior penalty virtual element method for the fourth-order elliptic hemivariational inequality
- [03325] Virtual element method for a frictional contact problem with normal compliance
- [03328] Well-posedness and Numerical Analysis of a Stokes Hemivariational Inequality
- [03157] Well-posedness of parabolic variational-hemivariational inequalities with unilateral constraints
- [03234] Duality Arguments in Analysis of Viscoelastic Contact Problem
- [03636] Frictional contact problem for electrorheological fluid flows
- [03327] Numerical analysis of history-dependent variational-hemivariational inequality by virtual element method
- [03250] Stability analysis for nonstationary Stokes hemivariational inequality

**[02616] Recent Developments in Applied Inverse Problems**

- [04397] Perturbation of Surface Waves in Piezoelectric Media
- [04646] Quantitative Parameter Reconstruction from Optical Coherence Tomographic Data
- [04241] Landweber-Kaczmarz for full datacube modelling in Extragalactic Archaeology

- [03014] Principles and Examples of Magnetic Resonance Elastography for Distribution Measurement of Viscoelasticity
- [04180] Inverse scattering technique for a defect in anisotropic plates
- [03045] Source Reconstruction from Partial Boundary Data in Radiative Transport
- [03961] Numerical challenges to optical tomography by the stationary radiative transport equation
- [04301] Inversion of the momenta X-ray transform of symmetric tensor fields in the plane.
- [02618] Recent Developments in Hyperspectral and Multispectral Imaging**
  - [03524] Multi-Dimensional Signal Alignment using Local All-Pass Filters
  - [03596] Noise reduction in X-ray microspectroscopy
  - [03540] Remote Sensing Image Reconstruction from the Subspace Perspective
  - [03879] Nonlocal Self-Similarity-Based Hyperspectral Remote Sensing Image Denoising With 3-D Convolutional Neural Network
- [02628] Mathematical Modeling on waste reduction through sustainable development.**
- [02644] Black box methods for efficient learning in high-dimensional scientific computing**
  - [05120] Is Monte Carlo a bad sampling strategy?
  - [05196] CAS4DL: Christoffel Adaptive Sampling for Deep Learning in data-scarce applications
  - [05283] Exploiting the local parabolic landscapes of adversarial losses to accelerate black-box adversarial attack
  - [05315] A Mathematical Approach Towards Physical Law Learning
- [02671] Recent advances on the analysis of hyperbolic balance laws**
  - [03611] Existence and Stability of Traveling Waves of Boussinesq-Burgers Equations
  - [04963] Global dynamics and photon loss in the Kompaneets equation
  - [03629] HYPOCOERCIVITY OF STOCHASTIC GALERKIN FORMULATIONS FOR STABILIZATION OF KINETIC EQUATIONS
  - [04154] Traveling Wave Solutions in Keller-Segel Models of Chemotaxis
  - [04448] On the Riccati dynamics of 2D Euler-Poisson equations with attractive forcing
  - [04918] Critical thresholds in spherically symmetric Euler-Poisson systems
  - [04518] On multi-dimensional rarefaction waves
  - [04947] Nonlocal traffic flow models
- [02700] Recent developments on Infinite Dimensional Analysis, Stochastic Analysis and Quantum Probability**
  - [02940] Note on complexities for the quantum compound systems
  - [03589] Asymptotics of densities of first passage times for spectrally negative Lévy processes
  - [03953] A combinatorial formula of the moments of a deformed field operator
  - [02981] Multiplication Operators by White Noise Delta Functions and Associated Differential Equations
  - [03986] Positivity of Q-matrices and quadratic embedding constants of graphs
  - [0,1]*i* f and only if the quadratic embedding constant (QEC) of G\$ is non-positive. We report some results in this line and discuss open questions.
- [03056] Data-driven methods to discover within-host biological dynamics**
  - [03279] How to find a pertinent research question: the identification and exploration of known unknowns
  - [05174] A summary of algorithms for sparse feature selection for Biological Data
  - [03409] Improving decoy detection for protein-protein interaction models
  - [05206] Early Detection of Disease: An intersection between artificial intelligence and biomathematics

## [00752] Theory and efficient methods for large-scale structured optimization models

**Session Time & Room :** 2E (Aug.22, 17:40-19:20) @D408

**Type :** Proposal of Minisymposium

**Abstract :** This mini-symposium is mainly on large-scale structured optimization models popular in statistical or machine learning community. We focus on the design of efficient algorithms for solving those large-scale structured optimization problems and the analysis of convergence theory of the proposed algorithms.

**Organizer(s) :** Yangjing ZHANG

**Classification :** 90C22, 90C46

**Minisymposium Program :**

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00752 (1/1) : 2E @D408 [Chair: Yangjing ZHANG]

## [01213] Augmented Lagrangian method for matrix optimization

**Format :** Talk at Waseda University

**Author(s) :** Chao Ding (Chinese Academy of Sciences)

**Abstract :** In this talk, we will introduce some new convergence results on the matrix optimization problems including nonlinear semidefinite programming and nonsmooth optimization on Riemannian manifold.

## [02195] Determinantal point processes for sampling minibatches in SGD

**Format :** Online Talk on Zoom

**Author(s) :** Rémi Bardenet (Université de Lille)Subhroshekhar Ghosh (National University of Singapore)Meixia Lin (Singapore University of Technology and Design)

**Abstract :** In this work, we contribute an orthogonal polynomial-based determinantal point process paradigm for performing minibatch sampling in SGD. Our approach leverages the specific data distribution at hand, which endows it with greater sensitivity and power over existing data-agnostic methods. We substantiate our method via a detailed theoretical analysis of its convergence properties, interweaving between the discrete data set and the underlying continuous domain. In particular, we show how specific DPPs and a string of controlled approximations can lead to gradient estimators with a variance that decays faster with the batchsize than under uniform sampling. Coupled with existing finite-time guarantees for SGD on convex objectives, this entails that, for a large enough batchsize and a fixed budget of item-level gradients to evaluate, DPP minibatches lead to a smaller bound on the mean square approximation error than uniform minibatches. Moreover, our estimators are amenable to a recent algorithm that directly samples linear statistics of DPPs without sampling the underlying DPP, thereby reducing computational overhead.

## [02194] Bregman Proximal Point Algorithm Revisited: A New Inexact Version and its Inertial Variant

**Format :** Talk at Waseda University

**Author(s) :** Lei Yang (Sun Yat-Sen University)Kim-Chuan Toh (National University of Singapore)

**Abstract :** In this talk, we focus on a general convex optimization problem, which covers various classic problems in different areas and particularly includes many optimal transport related problems arising in recent years. To solve this problem, we revisit the classic Bregman proximal point algorithm (BPPA) and introduce a new inexact stopping condition for solving the subproblems, which can circumvent the underlying feasibility difficulty often appearing in existing inexact conditions when the problem has a complex feasible set. Our inexact condition also covers several existing inexact conditions as special cases and hence makes our inexact BPPA (iBPPA) more flexible to fit different scenarios in practice. As an application to the standard optimal transport (OT) problem, our iBPPA with the entropic proximal term can bypass some numerical instability issues that usually plague the popular Sinkhorn's algorithm in the OT community. The iteration complexity of  $O(1/k)$  and the convergence of the sequence are also established for our iBPPA under some mild conditions. Moreover, inspired by Nesterov's acceleration technique, we develop an inertial variant of our iBPPA, denoted by V-iBPPA, and establish the iteration complexity of  $O(1/k^\lambda)$ , where  $\lambda \geq 1$  is a quadrangle scaling exponent of the kernel function. In particular, when the proximal parameter is a constant and the kernel function is strongly convex with Lipschitz continuous gradient (hence  $\lambda = 2$ ), our V-iBPPA achieves a faster rate of  $O(1/k^2)$  just as existing accelerated inexact proximal point algorithms. Some preliminary numerical experiments for solving the standard OT problem are conducted to show the convergence behaviors of our iBPPA and V-iBPPA under different inexactness settings. The experiments also empirically verify the potential of our V-iBPPA for improving the convergence speed.

## [02388] On efficient and scalable computation of the nonparametric maximum likelihood estimator in mixture models

**Format :** Talk at Waseda University

**Author(s) :** Yangjing ZHANG (Chinese Academy of Sciences)Ying Cui (University of Minnesota)Bodhisattva Sen (Columbia University)Kim-Chuan Toh (National University of Singapore)

**Abstract :** The nonparametric maximum likelihood estimation is a classic and important method to estimate the mixture models from finite observations. In this talk, we propose an efficient semismooth Newton based augmented Lagrangian method (ALM). By carefully exploring the structure of the ALM subproblem, we show that the computational cost of the generalized Hessian is independent of the number of grid points. Extensive experiments are conducted to show the effectiveness of our approach.

# [00753] Numerical methods for high-dimensional problems

**Session Time & Room :**

00753 (1/2) : 4C (Aug.24, 13:20-15:00) @G704

00753 (2/2) : 4D (Aug.24, 15:30-17:10) @G704

**Type :** Proposal of Minisymposium

**Abstract :** High-dimensional problems appear in various scientific areas and suffers from the notorious “curse of dimensionality” issue. This mini-symposium brings together the scientists working on quantum chemistry, classical and quantum kinetic theory and geophysics, etc., to share and exchanges their ideas in solving high-dimensional problems. Our mini-symposium will highlight the recent developments in both deterministic and particle-based methods. It is expected to elucidate the following questions: 1. Why do we need to solve high-dimensional problems? 2. What are common difficulties? 3. How to alleviate the curse of dimensionality by either novel mathematical methodologies or sophisticated usage of high-performance computing environment?

**Organizer(s) :** Yingzhou Li, Yunfeng Xiong

**Classification :** 35Q40, 35Q86, 82C05, 82C10, 65C20

**Minisymposium Program :**


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00753 (1/2) : 4C @G704 [Chair: Yingzhou Li]

## [04360] An efficient stochastic particle method for high-dimensional nonlinear PDEs

**Format :** Talk at Waseda University

**Author(s) :** Sihong Shao (Peking University)

**Abstract :** We introduce a stochastic particle method (SPM) to solve high-dimensional nonlinear PDEs in the weak sense. The weak formulation is a time-dependent high-dimensional integral, and different test functions can bring us various information about the solution. To determine the dynamics of the particle system, we linearize the nonlinear terms using the previous time step solutions and establish a relationship of weak formulation between adjacent time steps via the Lawson-Euler scheme. The resulting stochastic particles follow the behavior of the solution in an adaptive manner, therefore mitigating curse of dimensionality to a certain extent. Numerical experiments on the 6-D Allen-Cahn equation and 7-D Hamiltonian-Jacobi-Bellman equation demonstrate the accuracy and efficiency of SPM. This work is joint with Zhengyang Lei and Yunfeng Xiong.

## [04066] Overcoming the dynamical sign problem via adaptive particle annihilation

**Format :** Talk at Waseda University

**Author(s) :** Yunfeng Xiong (Beijing Normal University)

**Abstract :** The dynamical sign problem poses a fundamental obstacle to particle-based simulations in high dimensional space. To resolve it, we propose an adaptive particle annihilation algorithm, termed Sequential-clustering Particle Annihilation via Discrepancy Estimation (SPADE). SPADE follows a divide-and-conquer strategy: Adaptive clustering of particles via controlling their number-theoretic discrepancies and independent random matching in each cluster. Combining SPADE with the stationary phase approximation, we attempt to simulate the Wigner dynamics in 6-D and 12-D phase space.

## [02525] A splitting Hamiltonian Monte Carlo method for efficient sampling

**Format :** Talk at Waseda University

**Author(s) :** Lei Li (Shanghai Jiao Tong University) Lin Liu (Shanghai Jiao Tong University) Yuzhou Peng (Shanghai Jiao Tong University)

**Abstract :** In this talk, I will introduce a splitting Hamiltonian Monte Carlo algorithm, which can be computationally efficient when combined with the random mini-batch strategy. By splitting the potential energy into numerically nonstiff and stiff parts, one makes a proposal using the nonstiff part, followed by a Metropolis

rejection step using the stiff part that is often easy to compute. The splitting allows efficient sampling from systems with singular potentials and/or multiple potential barriers. We also use random batch strategies to reduce the computational cost in generating the proposals for problems arising from many-body systems and Bayesian inference, and estimate both the strong and the weak errors in the Hamiltonian induced by the random batch approximation.

## [02255] Ergodicity and sharp error estimate of Stochastic Gradient Langevin Dynamics

**Format :** Talk at Waseda University

**Author(s) :** Yuliang Wang (Shanghai Jiao Tong University)

**Abstract :** We establish a sharp error estimate for the Stochastic Gradient Langevin Dynamics (SGLD). Under mild assumptions, we obtain a uniform-in-time  $O(\eta^2)$  bound for the KL-divergence between SGLD and the Langevin diffusion, where  $\eta$  is the step size. Based on this, we are able to obtain an  $O(\eta)$  bound for its sampling error in terms of Wasserstein or total variation distances. Moreover, we prove the geometric ergodicity of SGLD algorithm under  $W_1$  distance without global convexity.

00753 (2/2) : 4D @G704 [Chair: Yunfeng Xiong]

## [04069] Multi-level Monte Carlo methods in stochastic density functional theory

**Format :** Talk at Waseda University

**Author(s) :** Huajie Chen (Beijing Normal University)

**Abstract :** The stochastic density functional theory (sDFT) has become an attractive approach in electronic structure calculations. The computational complexity of Hamiltonian diagonalization is replaced by introducing a set of random orbitals leading to sub-linear scaling of evaluating the ground-state observables. This work investigates the convergence and acceleration of the self-consistent field (SCF) iterations for sDFT in the presence of statistical error. We also study some variance reduction schemes by multi-level Monte Carlo methods that can accelerate the SCF convergence.

## [04185] Inchworm Monte Carlo Method for Spin Chain Models in Open Quantum Systems

**Format :** Talk at Waseda University

**Author(s) :** Zhenning Cai (National University of Singapore)

**Abstract :** We consider open quantum systems where the quantum system is coupled to a harmonic bath. When the coupling is weak, we can mimic Feynman's methodology to represent the dynamics as the sum of infinite integrals represented by diagrams. In this talk, we will discuss an efficient diagrammatic approach, known as the inchworm Monte Carlo method, to compute the observables in open quantum systems. Applications to spin chain models will be considered in the numerical tests.

## [04220] A short-memory operator splitting scheme for constant-Q viscoelastic wave equation

**Format :** Talk at Waseda University

**Author(s) :** Yunfeng Xiong (Beijing Normal University)Xu Guo (Shandong University)

**Abstract :** We propose a short-memory operator splitting scheme for solving the constant-Q wave equation, where the fractional stress-strain relation contains multiple Caputo fractional derivatives with order much smaller than 1. The key is to exploit its extension problem by converting the flat singular kernels into strongly localized ones, so that the major contribution of weakly singular integrals over a semi-infinite interval can be captured by a few Laguerre functions with proper asymptotic behavior. An operator splitting scheme is introduced to solve the resulting set of equations, where the auxiliary dynamics can be solved exactly, so that it gets rid of the numerical stiffness and discretization errors. Numerical experiments on both 1-D diffusive wave equation and 2-D constant-Q P-and S-wave equations are presented to validate the accuracy and efficiency of the proposed scheme.

## [04363] Solving Boltzmann equation with neural sparse representation

**Format :** Talk at Waseda University

**Author(s) :** Zhengyi Li (Peking Univeristy)Yanli Wang (Beijing Computational Science Research Center)Hongsheng Liu (Huawei Technologies Co. Ltd)Zidong Wang (Huawei Technologies Co. Ltd)Bin Dong (Beijing International Center for Mathematical Research & Center for Machine Learning Research, Peking University)

**Abstract :** We consider the neural sparse representation to solve Boltzmann equation. The different low-rank representations are utilized in the microscopic velocity for the BGK and quadratic collision model, resulting in a significant reduction in the degree of freedom. We approximate the discrete velocity distribution in the BGK model using the canonical polyadic decomposition. For the quadratic collision model, a data-driven, SVD-based linear basis is built based on the BGK solution.

## [00754] Regularization models and sampling algorithms in statistics and inverse problems

**Session Time & Room :**

00754 (1/2) : 1E (Aug.21, 17:40-19:20) @E503

00754 (2/2) : 2C (Aug.22, 13:20-15:00) @E503

**Type :** Proposal of Minisymposium

**Abstract :** Inverse problems involve the determination of unknown parameters from observational data and mathematical models linking those parameters to the data. Bayesian inference offers a framework to estimate the solution in terms of a posterior probability distribution. Oftentimes, the computation of the posterior requires application of Markov chain Monte Carlo (MCMC) methods. Direct implementation of these techniques becomes a challenge when the target parameters have a particular structure and are high-dimensional. This mini-symposium aims at presenting recent developments in sampling methods and prior/regularization models in statistics and inverse problems, including novel MCMC techniques, Monte Carlo estimators, and priors encoding structural information.

**Organizer(s) :** Felipe Uribe, Andreas Rupp

**Classification :** 62F15, 65C05, 65R32

**Minisymposium Program :**

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00754 (1/2) : 1E @E503 [Chair: Andreas Rupp]

## [03567] Efficient Bernoulli Factory MCMC

**Format :** Talk at Waseda University

**Author(s) :** Dootika Vats (Indian Institute of Technology Kanpur)Flávio Gonçalves (Universidade Federal de Minas Gerais)Krzysztof Łatuszyński (University of Warwick)Gareth Roberts (University of Warwick)

**Abstract :** Accept-reject based Markov chain Monte Carlo (MCMC) algorithms have traditionally utilised acceptance probabilities that can be explicitly written as a function of the ratio of the target density at the two contested points. This feature is rendered almost useless in Bayesian posteriors with unknown functional forms. We introduce a new family of MCMC acceptance probabilities that has the distinguishing feature of not being a function of the ratio of the target density at the two points. We present a stable Bernoulli factory that generates events within this class of acceptance probabilities. The efficiency of our methods rely on obtaining reasonable local upper or lower bounds on the target density and we present an application of MCMC on constrained spaces where this is reasonable.

## [03753] Sampling of Student's t and stable priors for edge-preserving Bayesian inversion

**Format :** Talk at Waseda University

**Author(s) :** Felipe Uribe (Lappeenranta-Lahti University of Technology)

**Abstract :** The identification of sharp features in the solution is a critical aspect of many large-scale Bayesian inverse problems. Markov random field (MRF) priors based on heavy-tailed distributions have proven effective in achieving piecewise constant behavior. This study reexamines the use of Student's t and alpha stable MRFs in this context. To facilitate computation of the resulting posterior distribution, we propose a scale mixture formulation of the MRF priors. This formulation has the advantage of expressing the prior as a conditionally Gaussian distribution that depends on auxiliary hyperparameters. We discuss a Gibbs sampler to solve the hierarchical formulation of the Bayesian inverse problem. The approach is illustrated using applications from imaging science.

## [04286] Comparison of pseudo-marginal Markov chains via weak Poincaré inequalities

**Format :** Talk at Waseda University

**Author(s) :** Andi Qi Wang (University of Warwick)Christophe Andrieu (University of Bristol)Anthony Lee (University of Bristol)Sam Power (University of Bristol)

**Abstract :** I will discuss the use of a certain class of functional inequalities known as weak Poincaré inequalities to bound convergence of Markov chains to equilibrium. This enables the straightforward and transparent derivation of subgeometric convergence bounds for methods such pseudo-marginal MCMC methods for intractable likelihoods, which have been used extensively in the context of Bayesian Inverse Problems.

## [04985] CUQIpy: Computational Uncertainty Quantification for Inverse Problems in Python

**Format :** Talk at Waseda University

**Author(s) :** Nicolai André Brogaard Riis (Technical University of Denmark)

**Abstract :** We present CUQIpy, a versatile open-source Python package for computational uncertainty quantification (UQ) in inverse problems using a Bayesian framework. This talk highlights CUQIpy's high-level modeling framework with concise syntax, enabling intuitive problem specification, and showcasing its efficient sampling strategies, automatic sampler selection, and test problem library. Designed to handle large-scale problems and support various probability distributions, CUQIpy streamlines the UQ process, serving as a powerful tool for a diverse set of inverse problems.

00754 (2/2) : 2C @E503 [Chair: Felipe Uribe]

## [05558] Gaussian likelihoods for non-Gaussian data

**Format :** Talk at Waseda University

**Author(s) :** Heikki Haario (University of Lappeenranta)

**Abstract :** Various modelling situations – chaotic dynamics, stochastic differential equations, random patterns by the Turing reaction-diffusion systems, cellular automata– share the analogy that a fixed model parameter corresponds to a family of solutions rather than a fixed deterministic one. This may be due to extreme sensitivity with respect to the initial values, randomized or unknown initial values, or explicit stochasticity of the system. Standard methods based on directly measuring the distance between model and data are no more available. We discuss a unified construction of Gaussian likelihoods for such ‘intractable’ situation, where the raw data is far from Gaussian. Examples cover the cases in the above list of modelling situations.

## [05515] Multi-output multilevel best linear unbiased estimators via semidefinite programming

**Format :** Talk at Waseda University

**Author(s) :** Matteo Croci (University of Texas at Austin)Karen E. Willcox (University of Texas at Austin)Stephen J. Wright (University of Wisconsin - Madison)

**Abstract :** Multifidelity forward uncertainty quantification (UQ) problems often involve multiple quantities of interest and heterogeneous models (e.g., different grids, equations, dimensions, physics, surrogate and reduced-order models). While computational efficiency is key in this context, multi-output strategies in multilevel/multifidelity methods are either sub-optimal or non-existent. In this talk we extend multilevel best

part\_2

linear unbiased estimators (MLBLUE) to multi-output forward UQ problems and we present new semidefinite programming formulations for their optimal setup. Not only do these formulations yield the optimal number of samples required, but also the optimal selection of low-fidelity models to use. While existing MLBLUE approaches are single-output only and require a non-trivial nonlinear optimization procedure, the new multi-output formulations can be solved reliably and efficiently. We demonstrate the efficacy of the new methods and formulations in practical UQ problems with model heterogeneity.

### [03923] Simulating rare events with Stein variational gradient descent

**Format :** Talk at Waseda University

**Author(s) :** Max Ehre (Technical University of Munich)Iason Papaioannou (Technical University of Munich)Daniel Straub (Technical University of Munich)

**Abstract :** Stein variational gradient descent (SVGD) is an approach to sampling from Bayesian posterior distributions. We repurpose SVGD for simulating rare events with probabilities  $10^{-5} \text{ -- } 10^{-12}$ . We employ a tempered version of SVGD to sample from an approximately optimal importance sampling density. Several examples are used to benchmark the efficacy of our approach against state-of-the-art methods for estimating rare event probabilities.

## [00760] Improving Reproducibility, Trustworthiness and Fairness in Machine Learning

**Session Time & Room :**

00760 (1/2) : 2C (Aug.22, 13:20-15:00) @E803

00760 (2/2) : 2D (Aug.22, 15:30-17:10) @E803

**Type :** Proposal of Minisymposium

**Abstract :** The widespread uptake of machine learning for completing routine and complex tasks has been an ambition that feels closer and closer every year. There is currently a well-known reproducibility crisis impacting machine learning-based science which could damage public confidence in the tools and hamper a rapid uptake. The diverse array of speakers in this minisymposium will present a range of talks focussing on practical solutions to different aspects of the reproducibility crisis, ways to address inequalities in algorithm performance to improve fairness, improving explainability of models, and methods to assess the robustness of algorithms.

**Organizer(s) :** Michael Roberts, Daniel Kreuter

**Classification :** 68T01, 68T07, 68P27, 92C50

**Minisymposium Program :**

00760 (1/2) : 2C @E803

### [01736] Improving reproducibility, trustworthiness and fairness for diverse applications of machine learning

**Author(s) :** Hirotaka Takahashi (Tokyo City University)

**Abstract :** Machine learning is applied to a diverse set of problems in our group. For example, research on gravitational wave physics and astronomy, development of traffic safety training and skills education methods, athlete support system of various sports, application to education to collaborate between teachers and machine learning etc.. In this presentation, we would like to focus on various applications and discuss how we can improve reproducibility, trustworthiness and fairness in machine learning.

## [01850] Multi-domain & Multi-task Generalisation on Real-World Clinical Data

**Author(s)** : Daniel Kreuter (University of Cambridge)Samuel Tull (University of Cambridge)

**Abstract** : Machine learning models have been holding the promise to revolutionise healthcare for several years. However, we rarely see promising approaches translate into deployment in the clinic. Often, this is due to an unexpected drop in performance when deploying the model on unseen test data due to domain shift. Our novel "Disentanglement Autoencoder" approach allows for multiple domains and tasks, both continuous and categorical, creating a disentangled embedding which can be used for multiple classification tasks.

## [01993] Classification of datasets with imputed missing values: does imputation quality matter?

**Author(s)** : Tolou Shadbahr (University of Helsinki)Michael Thomas Roberts (University of Cambridge)Jan Stanczuk (University of Cambridge)Julian Gilbey (University of Cambridge)Philip Teare (AstraZeneca)Sören Dittmer (University of Cambridge)MAthew Thorpe (University of Manchester)Ramon Vinas Torne (University of Cambridge)Evis Sala (University of Cambridge)Pietro Lio (University of Cambridge)Mishal Patel (AstraZeneca)James H.F. Rudd (University of Cambridge)Tuomas Mirtti (university of Helsinki)Antti Sakari Rannikko (university of Helsinki)John Aston (University of Cambridge)Jing Tang (University of Helsinki)Carola-Bibiane Schönlieb (University of Cambridge)

**Abstract** : Classifying samples in incomplete datasets is a common non-trivial task. Missing data is commonly observed in real-world datasets. Missing values are typically imputed, followed by classification of the now complete samples. Often, the focus is to optimize the downstream classification performance. In this talk, we highlight the serious consequences of using poorly imputed data, demonstrate how the common quality measures for measuring imputation quality are flawed, and introduce an improved class of imputation quality measures.

## [02088] A critical look: overly optimistic results on the TPEHGDB dataset

**Author(s)** : Gilles Vandewiele (IDLab, Ghent)

**Abstract** : I will discuss the overly optimistic prediction results that arise when applying oversampling on data before partitioning into a train and test set. Specifically, I will present a case study on predicting preterm birth using the TPEHG database where many studies report near-perfect predictive performances due to making a fundamental mistake. After correcting this mistake, the predictive power of the models becomes similar to a coin toss.

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00760 (2/2) : 2D @E803

## [02239] Software engineering for data science

**Author(s)** : Sören Dittmer (Uni Cambridge)

**Abstract** : Despite democratized data science tools, developing a trustworthy and effective data science system (DSS) is becoming increasingly challenging. The lack of software engineering (SE) skills and perverse incentives are among the root causes. We analyze why SE and building large complex systems, in general, is hard. We identify how SE addresses those difficulties and discuss how to adapt the insides to DSSs. We emphasize two key development philosophies: incremental growth and feedback loops.

## [02265] Leakage and the reproducibility crisis in ML-based science

**Author(s)** : Sayash Kapoor (Princeton University)Arvind Narayanan (Princeton University)

**Abstract** : As quantitative fields adopt ML methods, it is important to ensure reproducibility. We show that data leakage is a widespread problem and has led to severe reproducibility failures. Through a literature survey of research in communities that adopted ML methods, we show that errors have been found in 17 fields, collectively affecting hundreds of papers and leading to wildly overoptimistic conclusions. We propose model info sheets to detect and prevent leakage in ML-based science.

## [02340] ShearletX: A Mathematical Approach Towards Explainability

**Author(s)** : Gitta Kutyniok (LMU Munich)Stefan Kolek (LMU Munich)Robert Windesheim (LMU Munich)Hector Andrade Loarca (LMU Munich)Ron Levie (Technion)

**Abstract** : Automated decision making using machine learning, in particular deep learning, is becoming an increasingly important component of modern technical systems and often affects humans directly. In this talk, we will present an explainability approach, coined ShearletX, based on a combination of information theory and applied harmonic analysis, which not only often outperforms state-of-the-art methods, but is also accessible to a mathematical analysis.

## [02574] A tale of two crises: COVID-19 and ML reproducibility

**Author(s)** : Michael Thomas Roberts (University of Cambridge)

**Abstract** : Machine learning, like many fields before it, is suffering from a reproducibility crisis. In this talk we will give an overview of four different domains in which issues have been identified: (a) imaging, (b) missing data imputation, (c) learning at scale and (d) engineering of codebases. We also present solutions to problems identified.

# [00761] Recent Advances on quadrature methods for integral equations and their applications

**Session Time & Room :**

00761 (1/3) : 1C (Aug.21, 13:20-15:00) @A510

00761 (2/3) : 1D (Aug.21, 15:30-17:10) @A510

00761 (3/3) : 1E (Aug.21, 17:40-19:20) @A510

**Type** : Proposal of Minisymposium

**Abstract** : Numerical methods based on integral equations are powerful tools for simulating physical systems that arise in fluid mechanics, acoustics, electromagnetics, and many other fields. A crucial component of any efficient integral equation solver is a specialized quadrature method for the discretization of the underlying integral operators. This mini-symposium will focus on the main challenges in quadrature research including accurate evaluation of singular and near-singular integrals associated with surface and volume potentials, adaptive discretization in complex geometries, and the efficient implementation of quadrature schemes in practical applications.

**Organizer(s)** : Anna-Karin Tornberg, Hai Zhu, Bowei Wu

**Classification** : 65R20, 65N38

**Minisymposium Program :**

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00761 (1/3) : 1C @A510 [Chair: Bowei Wu]

## [04432] A High-Order Close Evaluation Scheme of Helmholtz Layer Potentials in 3D

**Format** : Talk at Waseda University

**Author(s)** : Hai Zhu (Flatiron Institute)Shidong Jiang (Flatiron Institute)

**Abstract** : We present an efficient high-order discretization scheme for the evaluation of the Helmholtz layer potentials on smooth surfaces in three dimensions. The scheme is panel based and applies an analytical surface to line integral conversion on each panel to evaluate single layer, double layer, adjoint double layer, and hypersingular potentials accurately. A new basis approximation scheme tailed for Helmholtz kernels is proposed. Both nearly singular and singular cases are supported via the same recursive framework.

## [04811] Special quadrature via line extrapolation, with application to Stokes flow

**Format :** Talk at Waseda University

**Author(s) :** Joar Bagge (KTH Royal Institute of Technology)Anna-Karin Tornberg (KTH Royal Institute of Technology)

**Abstract :** In integral equations, special quadrature methods are needed to perform singular or nearly singular integration. We consider one such method, sometimes called the "Hedgehog method", based on extrapolation (or interpolation) along a line. Different strategies for selecting the placement of sampling points along the line are investigated. We consider extrapolation using polynomials or rational functions. The resulting methods are compared with quadrature by expansion (QBX) in the context of Stokes flow containing rigid rodlike particles.

## [05076] Corrected trapezoidal rules for boundary integral methods on non-parametrized surfaces

**Format :** Talk at Waseda University

**Author(s) :** Olof Runborg (KTH Royal Institute of Technology)Richard Tsai (The University of Texas at Austin)Yimin Zhong (Auburn University )Federico Izzo (KTH Royal Institute of Technology)

**Abstract :** We present higher-order quadratures for a family of boundary integral operators with application to the linearized Poisson-Boltzmann equation. Using the Implicit Boundary Integral formulation, surface point singularities in a layer potential extend along the surface normal lines. In this volumetric setting, we use the trapezoidal rule, and develop higher-order quadratures by correcting it in nodes close to the singularity line with weights dependent on the singularity type and geometrical information extracted from the non-parametrized surface.

## [03610] Quadrature errors for layer potentials near surfaces with spherical topology

**Format :** Talk at Waseda University

**Author(s) :** Chiara Sorgentone (Sapienza, Università di Roma)Anna-Karin Tornberg (KTH Royal Institute of Technology)

**Abstract :** Numerical simulations often involve 3D objects with spherical topology, e.g. rigid particles, drops, vesicles. When the underlying numerical method is based on boundary integral equations, standard quadrature rules can yield large errors in computing the layer potentials if the distance between the surfaces is too small and the associated integrals become nearly singular. We will present numerical and analytical approaches to efficiently evaluate the quadrature error estimates for these situations.

00761 (2/3) : 1D @A510 [Chair: Anna-Karin Tornberg]

## [03612] Euler-Maclaurin formulas for near-singular integrals

**Format :** Talk at Waseda University

**Author(s) :** Bowei Wu (University of Massachusetts Lowell)

**Abstract :** Near-singular integrals frequently arise in fluid dynamics, material science, and many other scientific applications, where close fluid-structure interactions are common. Numerical approximation of near-singular integrals thus has practical importance. Approximating near-singular integrals using regular quadrature methods is in general inefficient and expensive. But more efficient quadrature rules can be developed by modifying regular quadrature rules using an error correction approach. We introduce new generalized Euler-Maclaurin formulas that are tailored to a family of near-singular functions. High-order accurate modified Trapezoidal quadrature rules are then derived based on these formulas.

## [03009] Near singularity errors in boundary integrals: identification, estimation and swapping

**Format :** Talk at Waseda University

**Author(s) :** Ludvig af Klinteberg (Mälardalen University)

**Abstract :** Evaluating a layer potential close to its source geometry poses numerical difficulties due to the presence of a near singularity. In this presentation I will discuss how the singularity can be understood in terms of its complexified preimage in the parametrization of the source geometry. Finding the preimage numerically allows us to both estimate quadrature errors to high precision, and derive new and more capable quadrature methods.

## [04640] An adaptive discretization technique for boundary integral equations in the plane

**Format :** Talk at Waseda University

**Author(s) :** Adrianna Gillman (University of Colorado, Boulder)Yabin Zhang (Westlake University)

**Abstract :** Typically the discretization of integral equations on two dimensional complex geometries involves the use of a panel based quadrature (such as variants of Gaussian quadrature). The placement of the panels is often ad hoc and based on being able to integrate quantities such as arc-length and/or curvature to a desired accuracy. These quantities do not necessarily correspond to what is needed to achieve accuracy in the solution to a partial differential equation. Alternatively, a refinement strategy based on looking at relative error and wisely choosing which part of the geometry to refine can be done but this involves global solves which can be prohibitively expensive. In this talk, we will present an adaptive discretization technique which is guaranteed to achieve the desired accuracy and does not require the inversion of a full discretized integral equation at each step in the refinement process. Numerical results will illustrate the performance of the method.

## [05159] A fully adaptive, high-order, fast Poisson solver for complex two-dimensional geometries

**Format :** Talk at Waseda University

**Author(s) :** Daniel Fortunato (Flatiron Institute)David B Stein (Flatiron Institute)Alex H Barnett (Flatiron Institute)

**Abstract :** We present a new framework for the fast solution of inhomogeneous elliptic boundary value problems in domains with smooth boundaries. High-order solvers based on adaptive box codes or the fast Fourier transform can efficiently treat the volumetric inhomogeneity, but require care to be taken near the boundary to ensure that the volume data is globally smooth. We avoid function extension or cut-cell quadratures near the boundary by dividing the domain into two regions: a bulk region away from the boundary that is efficiently treated with a truncated free-space box code, and a variable-width boundary-conforming strip region that is treated with a spectral collocation method and accompanying fast direct solver. Particular solutions in each region are then combined with layer potentials to yield the global solution. The resulting solver has an optimal computational complexity of  $O(N)$  for an adaptive discretization with  $N$  degrees of freedom. We demonstrate adaptive resolution of volumetric data, boundary data, and geometric features across a wide range of length scales, to typically 10-digit accuracy.

00761 (3/3) : 1E @A510 [Chair: Hai Zhu]

## [02383] Is polynomial interpolation in the monomial basis unstable?

**Format :** Talk at Waseda University

**Author(s) :** Zewen Shen (University of Toronto)Kirill Serkh (University of Toronto)

**Abstract :** Polynomial interpolation in the monomial basis is a key step in a number of popular quadrature methods for integral equations. We will show that, despite its ill-conditioning, the monomial basis is generally as good as a well-conditioned polynomial basis for interpolation, provided that the Vandermonde matrix has a condition number smaller than the reciprocal of machine epsilon. We will also explore some applications of our analysis.

## [04278] A new boundary integral equation solver for problems in exteriors of open arcs

**Format :** Talk at Waseda University

**Author(s) :** Abinand Gopal (Yale University)Shidong Jiang (Flatiron Institute )Vladimir Rokhlin (Yale University)

**Abstract :** When solving a constant-coefficient elliptic PDE, it is often convenient to first reformulate the problem as a boundary integral equation. This is usually done by representing the solution as an unknown density function times a kernel function integrated over the boundary of the domain. The choice of kernel is usually dictated by the

boundary conditions and made such that the resulting equation for the density is a second kind Fredholm integral equation.

However, when the problem is posed on the exterior of an arc in 2D or a surface in 3D, this becomes more complicated and the usual single layer and double layer representations run into difficulties. In this talk, we present a new solver for this regime. We use a representation based on the composition of standard layer potential with a hypersingular operator and compute the kernel of the composite operator directly. We then solve the resulting linear system with a direct solver.

## [04717] Density interpolation methods for volume integral operators

**Format :** Talk at Waseda University

**Author(s) :** Carlos Perez-Arancibia (University of Twente) Thomas G. Anderson (Rice University) Luiz M. Faria (INRIA/ENSTA Paris) Marc Bonnet (CNRS/ENSTA Paris)

**Abstract :** This talk outlines a novel class of high-order methods for the efficient numerical evaluation of volume potentials (VPs) defined by volume integrals over complex geometries. Inspired by the Density Interpolation Method (DIM) for boundary integral operators, the proposed methodology leverages Green's third identity and a local polynomial interpolation of the density function to recast a given VP as a linear combination of surface-layer potentials and a volume integral with a regularized (bounded or smoother) integrand. The layer potentials can be accurately and efficiently evaluated inside and outside the integration domain using existing methods (e.g. DIM), while the regularized volume integral can be accurately evaluated by applying elementary quadrature rules to integrate over structured or unstructured domain decompositions without local numerical treatment at and around the kernel singularity. The proposed methodology is flexible, easy to implement, and fully compatible with well-established fast algorithms such as the Fast Multipole Method and H-matrices, enabling VP evaluations to achieve linearithmic computational complexity. To demonstrate the merits of the proposed methodology, we applied it to the Nyström discretization of the Lippmann-Schwinger volume integral equation for frequency-domain Helmholtz scattering problems in piecewise-smooth variable media.

## [05303] Recursive product integration schemes for volume potentials on irregular domains

**Format :** Talk at Waseda University

**Author(s) :** shravan veerapaneni Hai Zhu (Flatiron Institute)

**Abstract :** We will discuss a new volume potential evaluation scheme for Gaussian and Laplace kernel in complex domains. The volume integral is computed by applying Green's theorem to convert these smooth or singular domain integrals on a volume mesh to a set of line integrals on the boundary skeleton of the volume mesh. This new approach allows easier integral-equation based solver implementation in complex domains, with much fewer restrictions on leaf level box refinement.

## [00763] Long-time dynamics of numerical methods for nonlinear evolution equations

**Session Time & Room :**

00763 (1/3) : 4C (Aug.24, 13:20-15:00) @E606

00763 (2/3) : 4D (Aug.24, 15:30-17:10) @E606

00763 (3/3) : 4E (Aug.24, 17:40-19:20) @E606

**Type :** Proposal of Minisymposium

**Abstract :** The numerical simulation of many physical systems requires an understanding of solutions which goes beyond mere numerical accuracy - they possess invariant structure and qualitative features that distinguish physically meaningful from spurious behaviour. This leads to the fundamental question to what extend such features of the underlying system can be preserved in the numerical flow, in particular over times much longer than is guaranteed by local error estimates. The proposed minisymposium brings together experts from computational mathematics to provide an overview of current state-of-the-art and recent advances in the study and design of methods for evolution equations with favourable long-time behaviour.

**Organizer(s) :** Yue Feng, Georg Maierhofer, Katharina Schratz

**Classification :** 65M15, 65M70, 35Q99, Long-time Dynamics, Geometric Numerical Integration, Error Analysis  
**Minisymposium Program :**

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00763 (1/3) : 4C @E606 [Chair: Yue Feng]

## [03792] Bourgain techniques for error estimates at low regularity

**Format :** Talk at Waseda University

**Author(s) :** Alexander Ostermann (Universität Innsbruck)Lun Ji (Universität Innsbruck)Frédéric Rousset (Université Paris-Saclay)Katharina Schratz (Sorbonne Université)

**Abstract :** Standard numerical integrators suffer from order reduction when applied to nonlinear dispersive equations with non-smooth initial data. For such problems, we present filtered integrators that exhibit superior convergence rates at low regularity. Furthermore, due to the nonexistence of suitable embedding results, the error analysis at very low regularity cannot be carried out in standard Sobolev spaces. Instead, new techniques are required. They are based on Bourgain's seminal work and will be sketched in the talk.

## [01832] Improved uniform error bounds of the time-splitting methods for the long-time (nonlinear) Schrödinger equation

**Format :** Talk at Waseda University

**Author(s) :** Yue Feng (Laboratoire Jacques-Louis Lions)

**Abstract :** In this talk, I will present the improved uniform error bounds of the time-splitting Fourier pseudospectral methods for the long-time dynamics of the Schrödinger equation with small potential and the nonlinear Schrödinger equation with weak nonlinearity. The main technique introduced is the regularity compensation oscillation (RCO), which control the high frequency modes by the regularity of the exact solution and the low frequency modes by phase cancellation and energy method.

## [04274] A symmetric low-regularity approximation to the nonlinear Schrödinger equation

**Format :** Talk at Waseda University

**Author(s) :** Yvonne Alama Bronsard (Sorbonne Université, LJLL)

**Abstract :** In this talk we will discuss the approximation to nonlinear dispersive equations which ask for low-regularity assumptions on the initial data, both for deterministic and random initial data.

We will put forth a novel time discretization to the nonlinear Schrödinger equation which allows for low-regularity approximation while maintaining good long-time preservation of the density and energy on the discrete level

## [04742] Symmetric low regularity integrators via a forest formula

**Format :** Talk at Waseda University

**Author(s) :** Yvain Bruned (Université de Lorraine)

**Abstract :** In this work, we will present general low regularity schemes that should encompass some of the symmetries of a given dispersive PDEs. We extend the low resonance decorated trees approach to a richer framework where we explore different ways of iterating Duhamel's formula and interpolating the lower part of the resonance for a Taylor approximation. This gives more degrees of freedom, encapsulated via a new forest formula that provides the general form for these new schemes. From this formula, we are able to derive conditions on the coefficients for finding new symmetric schemes. We believe that such an approach could tackle other symmetries.

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00763 (2/3) : 4D @E606 [Chair: Georg Maierhofer]

## [04423] Quantum computation of partial differential equations

**Format :** Talk at Waseda University

**Author(s) :** Shi Jin (Shanghai Jiao Tong University)

**Abstract :** Quantum computers have the potential to gain algebraic and even up to exponential speed up compared with its classical counterparts, and can lead to technology revolution in the 21st century. Since quantum computers are designed based on quantum mechanics principle, they are most suitable to solve the Schrödinger equation, and linear PDEs (and ODEs) evolved by unitary operators. The most efficient quantum PDE solver is quantum simulation based on solving the Schrödinger equation. It became challenging for general PDEs, more so for nonlinear ones. Our talk will cover two topics:

1. We introduce the “warped phase transform” to map general linear PDEs and ODEs to Schrodinger equation or with unitary evolution operators in higher dimension so they are suitable for quantum simulation;
2. For (nonlinear) Hamilton-Jacobi equation and scalar nonlinear hyperbolic equations we use the level set method to map them—exactly—to phase space linear PDEs so they can be implemented with quantum algorithms and we gain quantum advantages for various physical and numerical parameters.

## [05333] Asymptotic expansions for the linear PDEs with oscillatory input terms: Analytical form and error analysis

**Format :** Talk at Waseda University

**Author(s) :** Karolina Joanna Kropielnicka (Institute of Mathematics of Polish Academy of Sciences)

**Abstract :** Partial differential equations with highly oscillatory input term are hardly ever solvable analytically and they are difficult to treat numerically. Modulated Fourier expansion used as an ansatz is a well known and extensively investigated tool in asymptotic numerical approach for this kind of problems.

In this talk I will consider input term with single frequency and will show that the ansatz need not be assumed – it can be derived naturally while developing formulas for expansion coefficients. Moreover I will present the formula describing the error term and its estimates. Theoretical investigations will be illustrated by results of the computational simulations.

## [03756] A new picture on the Strang Splitting

**Format :** Talk at Waseda University

**Author(s) :** Juan Del Valle (University of Gdansk) Karolina Kropielnicka (Polish Academy of Sciences)

**Abstract :** Strang splitting is a well-established and widely used technique for finding approximate solutions of linear differential equations of the type  $u' = (A+B)u$ , where A and B are time-independent components. However, it can also be used for the case of time-dependent component B(t) after the application of the mid-point quadrature rule at the level of the Magnus expansion. However, the error estimate is absent in the case of singular cases of unbounded operators B(t).

In this talk, I will show how Strang splitting scheme for time-dependent components can be derived using the Duhamel formula. Based on this approach, I will (i) present a new proof of convergence of this scheme and (ii) elaborate on the possibilities brought by this approach for higher order methods. A concrete analysis of the error estimated and numerical simulations will be presented for the physically relevant example of a hydrogen atom featuring the singular Coulomb potential.

## [05308] The role of breathers in the formation of extreme ocean waves

**Format :** Talk at Waseda University

**Author(s) :** Amin Chabchoub (Kyoto University )

**Abstract :** The modulation instability is a fundamental mechanism, which explains localized wave focusing processes in dispersive wave systems. When considering the nonlinear Schrödinger equation as underlying wave model, exact breather solutions are particularly useful to initiate and control unstable wave dynamics in a numerical or laboratory experiment. This talk will summarize the main experimental achievements on breathers and connect these findings to the dynamics of ocean rogue waves.

00763 (3/3) : 4E @E606 [Chair: Georg Maierhofer]

## [04908] Structure-preserving finite element discretization of nonlinear PDEs

**Format :** Talk at Waseda University

**Author(s) :** Ari Stern (Washington University in St. Louis)

**Abstract :** This talk discusses some recent advances in structure-preserving methods for nonlinear PDEs, combining finite elements in space and geometric integration in time. In particular, we extend some earlier methods and results to a broader class of Hamiltonian PDEs than previously considered, showing that multisymplectic and other conservation laws are preserved. These methods apply on unstructured meshes, not just structured grids, and may be arbitrarily high-order.

## [01990] High-order mass- and energy-conserving methods for the nonlinear Schrödinger equation

**Format :** Talk at Waseda University

**Author(s) :** Genming Bai (The Hong Kong Polytechnic University) Jiashun Hu (The Hong Kong Polytechnic University) Buyang Li (The Hong Kong Polytechnic University)

**Abstract :** A class of high-order mass- and energy-conserving methods is proposed for the nonlinear Schrödinger equation based on Gauss collocation in time and finite element discretization in space, by introducing a mass- and energy-correction post-process at every time level. The existence, uniqueness and high-order convergence of the numerical solutions are proved. In particular, the error of the numerical solution is  $O(\tau^{k+1} + h^p)$  in the  $L^\infty(0, T; H^1)$  norm after incorporating the accumulation errors arising from the post-processing correction procedure at all time levels, where  $k$  and  $p$  denote the degrees of finite elements in time and space, respectively, which can be arbitrarily large. Several numerical examples are provided to illustrate the performance of the proposed new method, including the conservation of mass and energy, and the high-order convergence in simulating solitons and bi-solitons.

## [03931] Geometric two-scale integrators for highly oscillatory system

**Format :** Talk at Waseda University

**Author(s) :** Bin Wang (Xi'an Jiaotong University)

**Abstract :** In this talk, we consider a class of highly oscillatory Hamiltonian systems which involve a scaling parameter. We apply the two-scale formulation approach to the problem and propose two new time-symmetric numerical integrators. The methods are proved to have the uniform second order accuracy at finite times and some near-conservation laws in long times.

## [03985] Structure preserving schemes for Allen--Cahn type equations

**Format :** Talk at Waseda University

**Author(s) :** Yongyong Cai (Beijing Normal University)

**Abstract :** In comparison with the Cahn--Hilliard equation, the classic Allen--Cahn equation satisfies the maximum bound principle (MBP) but fails to conserve the mass. Here, we report the MBP and corresponding numerical schemes for the Allen--Cahn equation with nonlocal constraint for the mass conservation. As an extension, we discuss the case of the convective Allen--Cahn equation.

## [00766] Deep learning techniques for inverse problems and imaging

**Session Time & Room :** 5D (Aug.25, 15:30-17:10) @G808

**Type :** Proposal of Minisymposium

**Abstract :** Inverse problems involve identifying parameters of interest from indirect data. A main challenge for solving inverse problems is that their solutions are often not well posed, i.e., not unique and/or unstable with respect to small perturbations in the data. Deep techniques have been successfully applied to a wide variety of inverse problems, especially those arising in medical imaging. The main purpose of this mini-symposium is to discuss recent developments of the deep learning techniques for solving inverse problems and the open challenges that need to be addressed in the future.

**Organizer(s) :** Jinglai Li, Xiaoqun Zhang

**Classification :** 35R30, 68T07, 92C55

**Minisymposium Program :**

00766 (1/1) : 5D @G808

## [03603] Deep learning-based medical image reconstruction from incomplete data

**Format :** Online Talk on Zoom

**Author(s) :** Qiaoqiao Ding (Shanghai Jiao Tong University)

**Abstract :** Image reconstruction from down-sampled and corrupted measurements, such as fast MRI and sparse-view/low-dose CT, is mathematically ill-posed inverse problem. Deep neural network (DNN) has been becoming a prominent tool in the recent development of medical image reconstruction methods. In this talk, I will introduce our work on incorporating classical image reconstruction method and deep learning methods. The experiments on both sparse-view CT and low-dose CT problem show that the proposed method provided state-of-the-art performance.

## [05360] Deep Unrolling Networks with Recurrent Momentum Acceleration

**Format :** Talk at Waseda University

**Author(s) :** Qingping Zhou (School of Mathematics and Statistics, Central South University)Junqi Tang (School of Mathematics, University of Birmingham)Jinglai Li (School of Mathematics, University of Birmingham)

**Abstract :** Leveraging model-based iterative algorithms and deep learning, deep unrolling networks (DuNets) address inverse imaging problems. However, nonlinear problems hinder their efficacy. Our proposed recurrent momentum acceleration (RMA) framework employs a LSTM-RNN to simulate momentum acceleration, enhancing DuNets' performance. Applied to the learned proximal gradient descent (LPGD) and the learned primal-dual (LPD) methods, it results in LPGD-RMA and LPD-RMA, respectively. Experimental results on nonlinear deconvolution and electrical impedance tomography indicate significant improvements, particularly for strongly ill-posed problems.

## [05368] Spatiotemporal Imaging with Diffeomorphic Optimal Transportation

**Format :** Talk at Waseda University

**Author(s) :** Chong Chen (Academy of Mathematics and Systems Science, Chinese Academy of Sciences)

**Abstract :** This talk introduces a concept called diffeomorphic optimal transportation (DOT), which combines the Wasserstein distance with Benamou--Brenier formula in optimal transportation and the flow of diffeomorphisms in large deformation diffeomorphic metric mapping. Using DOT, a new variational model for joint image reconstruction and motion estimation is proposed, which is suitable for spatiotemporal imaging involving mass-preserving large diffeomorphic deformations. The performance is validated by several numerical experiments in spatiotemporal tomography.

## [05387] Self-supervised deep learning for imaging

**Format :** Talk at Waseda University

**Author(s) :** Hui Ji (National University of Singapore)

**Abstract :** Deep learning has proved to be a powerful tool in many domains, including inverse imaging problems. However, most existing successful deep learning solutions to these inverse problems are based on supervised learning, which requires many ground-truth images for training a deep neural network (DNN). This prerequisite on training datasets limits their applicability in data-limited domains, such as medicine and science. In this talk, we will introduce a series of works on self-supervised learning for solving inverse imaging problems. Our approach teaches a DNN to predict images from their noisy and partial measurements without seeing any related truth image, which is achieved by neuralization of Bayesian inference with DNN-based over-parametrization of images. Surprisingly, our proposed self-supervised method can compete well against supervised learning methods in many real-world imaging tasks..

# [00768] Recent Advances in Computational Tools of Scientific Machine Learning towards Digital Twins

## **Session Time & Room :**

00768 (1/2) : 2C (Aug.22, 13:20-15:00) @E818

00768 (2/2) : 2D (Aug.22, 15:30-17:10) @E818

**Type :** Proposal of Minisymposium

**Abstract :** Scientific Machine Learning is a new discipline that integrates traditional scientific computing and modern machine learning. It has grown explosively in recent years and is recognized as a fundamental research field that develops computational tools enabling Digital Twins. This mini-symposium will highlight recent progress in scientific machine learning techniques for Digital Twins and gather experts working on theory, algorithms, and applications to discuss and identify urgent current agendas and challenges.

**Organizer(s) :** Yeonjong Shin, Xueyu Zhu

**Classification :** 68Txx, 65Zxx, 65Yxx

## **Minisymposium Program :**

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00768 (1/2) : 2C @E818

## [03527] Digital Twins and Machine Learning from an Inverse Problem Perspective

**Author(s) :** Mark Asch (Université de Picardie Jules Verne)

**Abstract :** Digital Twins that are exchanging data with their real-world counterparts can be considered as instances of inverse problems—either of parameter identification type (static, or quasi-static), or of data assimilation type (dynamic). Many classical methods exist for solving inverse problems, but inverse problems remain complex, time-consuming and difficult to solve, especially with limited resources. However, machine learning can also be viewed as a parameter identification inverse problem, where for example in a neural network we seek to identify the weights (parameters) of the network. Moreover, the machine learning community has developed extremely efficient frameworks and tools for solving their inverse problems, such as stochastic gradient, backpropagation, and others. In this talk I will review machine learning methods with respect to the solution of inverse problems and I will present some examples of Digital Twins that have been developed on this basis.

## [03528] Physics-guided data-driven simulations for a digital twin

**Author(s) :** Youngsoo Choi (Lawrence Livermore National Laboratory)

**Abstract :** A computationally expensive physical simulation is a huge bottleneck for a digital twin. Fortunately, many data-driven approaches have emerged to accelerate those simulations, thanks to the recent advance in machine learning (ML) and artificial intelligence. For example, a well-trained 2D convolutional deep neural network can predict the solution of complex Richtmyer–Meshkov instability problem with a speed-up of 100,000x (1). However, the traditional black-box ML models do not incorporate existing governing equations, which embed underlying physics, such as conservation of mass, momentum, and energy. Therefore, the black-box ML models often violate important physics law, which greatly concerns physicists, and require big data to compensate the missing physics information. Additionally, it comes with other disadvantages, such as non-structure-preserving, computationally expensive training phase, non-interpretability, and vulnerability in extrapolation. To resolve these issues, we can bring physics into data-driven framework. Physics can be incorporated in different stages of data-driven modeling, i.e., sampling stage and model-building stage. Physics-informed greedy sampling procedure minimizes the number of required training data for a target accuracy (2). Physics-guided data-driven model better preserves physical structure and more robust in extrapolation than traditional black-box ML models. Numerical results, e.g., hydrodynamics (3,4), particle transport (5), plasma physics, and 3D printing, will be shown to

demonstrate the performance of the data-driven approaches. The benefits of the data-driven approaches will also be illustrated in multi-query decision-making applications, such as design optimization (6,7).

#### Reference:

- (1) Jekel, Charles F., Dane M. Sterbentz, Sylvie Aubry, Youngsoo Choi, Daniel A. White, and Jonathan L. Belof. "Using Conservation Laws to Infer Deep Learning Model Accuracy of Richtmyer-meshkov Instabilities." arXiv preprint arXiv:2208.11477 (2022).
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- (3) Copeland, Dylan Matthew, Siu Wun Cheung, Kevin Huynh, and Youngsoo Choi. "Reduced order models for Lagrangian hydrodynamics." Computer Methods in Applied Mechanics and Engineering 388 (2022): 114259.
- (4) Kim, Youngkyu, Youngsoo Choi, David Widemann, and Tarek Zohdi. "A fast and accurate physics-informed neural network reduced order model with shallow masked autoencoder." Journal of Computational Physics 451 (2022): 110841.
- (5) Choi, Youngsoo, Peter Brown, William Arrighi, Robert Anderson, and Kevin Huynh. "Space-time reduced order model for large-scale linear dynamical systems with application to boltzmann transport problems." Journal of Computational Physics 424 (2021): 109845.
- (6) McBane, Sean, and Youngsoo Choi. "Component-wise reduced order model lattice-type structure design." Computer methods in applied mechanics and engineering 381 (2021): 113813.
- (7) Choi, Youngsoo, Gabriele Boncoraglio, Spencer Anderson, David Amsallem, and Charbel Farhat. "Gradient-based constrained optimization using a database of linear reduced-order models." Journal of Computational Physics 423 (2020): 109787.

## [03532] Attributing anomalies from black-box predictions

**Author(s)** : Tsuyoshi Ide (IBM Research)

**Abstract** : One of the most important problems with digital twins is how to explain an unusual event observed as a significant discrepancy from the prediction of an AI model. Although this problem encompasses various different scenarios, we are particularly interested in the task of anomaly attribution in the black-box regression setting. The question is how we can quantify the contribution of each input variable in the face of an unexpected deviation between observation and prediction.

In this talk, I will first review existing attribution approaches recently developed in the machine learning community, including linear surrogate modeling, Shapley values, and integrated gradient. After summarizing the challenges of these methods in the particular context of anomaly explanation, I will touch upon a newer notion of likelihood compensation as one of the major counterfactual-type explanations. If time permits, I will share some experimental results, including the one conducted for IBM IoT Business Unit.

## [03536] AI Based Medical Twin System: Investigation on Focused Ultrasound Therapeutics

**Author(s)** : Kyungho Yoon (Yonsei University)

**Abstract** : In the huge paradigm shift of 4th industrial revolution driven by AI technique, the medical industry is also pursuing personalized precision medicine through digital transformation and smart transformation from analogue, standard, and empirical medical procedure. At the center of this change, IT technology is acting as key driving force. In particular, personalized digital twin model of human body and therapeutic tool will be the core engine of smart medicine. In this presentation, I will introduce research on the development of artificial intelligence-based medical twin systems for digital/smart therapeutics by convergence of computational science, medical engineering, and artificial intelligence technologies as the core technologies of the 4th medical revolution. In particular, investigation on the focused ultrasound device will be presented, which has recently been emerging as a non-invasive brain stimulation tool.

00768 (2/2) : 2D @E818

## [03635] Learning reduced-order operators with Bayesian inference and Gaussian processes

**Author(s)** : Mengwu Guo (University of Twente)

**Abstract** : Credible real-time simulation is a critical enabling factor for digital twin technology, and data-driven model reduction is a natural choice for achieving it. In this talk, we will discuss a probabilistic strategy for the learning of reduced-order representations of high-dimensional dynamical systems, with which a significantly reduced dimensionality guarantees improved efficiency, and the endowed uncertainty quantification certifies computational reliability. The strategy is based on Bayesian reduced-order operator inference, a data-driven part\_2

method that inherits the formulation structure of projection-based reduced-state governing equations yet without requiring access to full-order solvers. The reduced-order operators are estimated using Bayesian inference with Gaussian priors, and two fundamentally different strategies of likelihood definition will be discussed – one formulated as linear regression, and the other through Gaussian processes. Given by posterior Gaussian distributions conditioning on solution data, the reduced-order operators probabilistically define a low-dimensional dynamical system for the predominant latent states, and provide an inherently embedded Tikhonov regularization together with a quantification of modeling uncertainties.

## [04330] Operator learning for stochastic closures of complex dynamical systems

**Author(s)** : Jinlong Wu (University of Wisconsin-Madison)Chuanqi Chen (University of Wisconsin-Madison)

**Abstract** : Closure models are widely used in simulating complex multiscale dynamical systems such as turbulence and Earth's climate, for which direct numerical simulation that resolves all scales is often too expensive. For those systems without a clear scale separation, deterministic and local closure models often lack enough generalization capability, which limits their performance in many real-world applications. In this talk, we present a data-driven modeling framework for constructing stochastic and nonlocal closure models from (i) abundant data, and (ii) a limited amount of data. Specifically, operator learning with indirect data will be demonstrated in the context of stochastic differential equations. We also show how different types of regularization can be imposed to improve the performance of the learned closure models. The results show that the proposed methodology provides a systematic approach to constructing generalizable data-driven closure models for multiscale dynamical systems even if there is no clear scale separation between resolved and unresolved scales.

## [05255] ClimaX: A foundation model for weather and climate

**Author(s)** : Johannes Brandstetter (Microsoft Research)

**Abstract** : Most state-of-the-art approaches for weather and climate modeling are based on physics-informed numerical models of the atmosphere. These approaches aim to model the non-linear dynamics and complex interactions between multiple variables, which are challenging to approximate. Additionally, many such numerical models are computationally intensive, especially when modeling the atmospheric phenomenon at a fine-grained spatial and temporal resolution. Recent data-driven approaches based on machine learning instead aim to directly solve a downstream forecasting or projection task by learning a data-driven functional mapping using deep neural networks. However, these networks are trained using curated and homogeneous climate datasets for specific spatiotemporal tasks, and thus lack the generality of numerical models. We develop and demonstrate ClimaX, a flexible and generalizable deep learning model for weather and climate science that can be trained using heterogeneous datasets spanning different variables, spatio-temporal coverage, and physical groundings. ClimaX extends the Transformer architecture with novel encoding and aggregation blocks that allow effective use of available compute while maintaining general utility. ClimaX is pre-trained with a self-supervised learning objective on climate datasets derived from CMIP6. The pre-trained ClimaX can then be fine-tuned to address a breadth of climate and weather tasks, including those that involve atmospheric variables and spatio-temporal scales unseen during pretraining. Compared to existing data-driven baselines, we show that this generality in ClimaX results in superior performance on benchmarks for weather forecasting and climate projections, even when pretrained at lower resolutions and compute budgets.

## [00774] Applications of machine learning to analyzing time-series and imaging data

**Session Time & Room :**

00774 (1/2) : 2C (Aug.22, 13:20-15:00) @E817

00774 (2/2) : 2D (Aug.22, 15:30-17:10) @E817

**Type** : Proposal of Minisymposium

**Abstract** : Considerable increases in GPU and high-performance computing have led to significant advances in machine learning methodologies. This mini-symposium will focus on recent advances in methodologies and applications of deep and machine learning to analyze two types of data. In the first session, our speakers will discuss recent advances in machine learning based methods for predicting time series data. The second session will focus on deep learning for analyzing and interpreting imaging data. Mathematical topics of this mini symposium

include, but are not limited to, physics-driven machine learning, deep learning, reinforcement learning, computer vision, and optimal transport.

**Organizer(s)** : Kevin Flores, Ryan Murray, Hien Tran

**Classification** : 68T07, 49Q22, 65D19, 92B20

**Minisymposium Program :**

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00774 (1/2) : 2C @E817

## [03788] Predicting Bladder Pressure and Contractions from Non-Invasive Time-Series Data

**Author(s)** : Erica M Rutter (University of California, Merced)

**Abstract** : Symptoms of bladder dysfunction can be alleviated by electrical stimulation of nerves at the start of a contraction. However, determining when a bladder contraction will occur remains an active area of research. Due to the extremely dense time-series data, we employ statistical and machine learning methods to predict bladder pressure from external nerve data. These bladder pressures are used to predict the onset of bladder contractions with high sensitivity and specificity.

## [04294] Leveraging topological data analysis for parameter estimation of an agent-based model of collective motion

**Author(s)** : Kyle Nguyen (North Carolina State University) Carter Jameson (North Carolina State University) John Nardini (The College of New Jersey) Kevin Flores (North Carolina State University)

**Abstract** : Understanding the social interaction between members of groups in the context of collective motion is significant to gain the insights on the link between local and global behaviors. By leveraging topological data analysis, we use dimensional reduction techniques on topological features to visually cluster different time series of collective motion simulations of an agent-based model into groups. We also propose inverse problem approaches for parameter estimation of this particular agent-based model of collective motion.

## [04425] Few-Shot Learning for Leaf and Vein Segmentation

**Author(s)** : John Lagergren (Oak Ridge National Laboratory)

**Abstract** : Plant phenotyping is a primary bottleneck in understanding plant adaptation and the genetic architectures underlying complex traits at population scale. We address this challenge by leveraging few-shot learning with convolutional neural networks (CNNs) to segment the leaf body and visible venation of *P. trichocarpa* leaf images obtained in the field. Biological traits are extracted from the resulting segmentations, validated using real-world measurements, and used to conduct a genome-wide analysis to identify genes controlling the traits.

## [04513] Analysis of spatial transcriptomics using deep learning and optimal transport

**Author(s)** : Zixuan Cang (North Carolina State University)

**Abstract** : The emerging single-cell and spatial genomics techniques allow us to elucidate the governing rules of multicellular systems with unprecedented resolution and depth. These datasets are often high-dimensional, complex, and heterogeneous. Mathematical tools are needed to extract biological insights from such data. In this talk, we will discuss several computational methods for exploring tissue structures, temporal signatures, and cell-cell communication processes on spatial transcriptomics data as well as supervised optimal transport motivated by the biological applications.

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00774 (2/2) : 2D @E817

## [04520] Applied Machine Learning for Overhead Imagery

**Author(s)** : Adam Attarian (Pacific Northwest National Laboratory)

**Abstract** : Applying machine learning techniques to collected overhead imagery presents many challenges not normally encountered in traditional object detection and classification problems. Complex sensing geometries, small target size, and lack of sufficient training data are all problems that must be mitigated. In this talk, we provide an overview of machine learning approaches and techniques to derive meaningful information from overhead imagery.

## [04949] Introduction to miniympoium session: Applications of machine learning to analyzing time-series and imaging data

**Author(s)** : Kevin Flores (NC State University)

**Abstract** : This talk is an introduction to the minisymposium session on "Applications of machine learning to analyzing time-series and imaging data".

## [05230] Reinforcement Learning in a Digital Twin Framework for the Stabilization of an Inverted Pendulum

**Author(s)** : Hien Tran (North Carolina State University)

**Abstract** : In this talk we benchmark common reinforcement learning algorithms on a modified version of OpenAI Gym's Cartpole: a virtual environment simulating the dynamics of an inverted pendulum. The reinforcement learning algorithms that we used to stabilize the virtual inverted pendulum included the Policy Gradient, Actor-Critic, and Proximal Policy Optimization. We then transferred the trained neural network models from the virtual environment to the real physical inverted pendulum to verify their performances. While all of the reinforcement learning algorithms were able to satisfactorily balance the real inverted pendulum, Actor-Critic is best able to adequately reject disturbances.

## [05238] Solving inverse and forward problems in the water quality model by neutral networks

**Author(s)** : Quy Muoi Pham (The University of Danang - University of Science and Education)

**Abstract** : In this talk, we study the forward and inverse problems in BOD-DO models and present the Physic Inform Neural Network method to solve these problems. We first introduce the fully deep neural network and some well-known results about the approximation of fully deep neural networks to functions of classes. Then, we present the Physic Inform Neural Network method to solve the forward and inverse problems in BOD-DO models. We apply the method to solve some specific numerical examples. The method can be generalized for complex river quality models, e.g., 2D or 3D BOD-DO models or river quality models with more than two indicators. For complex river systems, we can use segmentation techniques to divide the river into some segments and in each segment, we can use the proposed method to solve the forward and inverse problems.

## [00778] Analysis, Applications, and Advances in Metamaterials and Composites

**Session Time & Room :**

00778 (1/3) : 4E (Aug.24, 17:40-19:20) @G801

00778 (2/3) : 5B (Aug.25, 10:40-12:20) @G801

00778 (3/3) : 5C (Aug.25, 13:20-15:00) @G801

**Type** : Proposal of Minisymposium

**Abstract** : Composites are inhomogeneous mixtures of their component materials. Metamaterials are composites with properties that go beyond those of the constituent phases and possibly beyond naturally occurring materials. These have attracted increasing attention in the past twenty years. Many important mathematical questions have been addressed, yet many remain. For example, composites and metamaterials can guide fields and waves in desired ways, e.g., cloaking, but the limitations of this are not so clear. Also, what unusual effective behaviors are possible? Incorporating dispersion, dissipation, anisotropy, extreme moduli, etc. adds to the challenge. This minisymposium will present exciting new developments in the field.

**Organizer(s)** : Maxence Cassier (CNRS, Institut Fresnel), Graeme W. Milton (University of Utah), Anthony Stefan (Florida Institute of Technology), Aaron Welters (Florida Institute of Technology)

**Classification** : 35Qxx, 74Qxx, 35B27, 78M40, 35R30, metamaterials, cloaking, active and passive media, dynamic materials, effective equations

**Minisymposium Program :**

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00778 (1/3) : 4E @G801 [Chair: Graeme Milton]

## [03353] Double-Zero-Index metamaterials

**Format :** Talk at Waseda University

**Author(s) :** Ying Wu (KAUST)Changqing Xu (KAUST)Keqiang Lyu (KAUST)Guancong Ma (Hong Kong Baptist University)Yun Lai (Nanjing University)

**Abstract :** Wave propagating in a medium with two constitutive parameters vanishing (double-zero index media) does not accumulate any phase retardation. Such a medium is not mathematically interesting but also bears unusual functionalities, such as wave front engineering, cloaking of objects and wave tunnelling. I will report our progresses on realizing double-zero index materials in two and three dimensions for electromagnetic and acoustic waves and discuss their special characteristics.

## [04938] Rigidity and Elasticity of Kirigami and Origami Metamaterials

**Format :** Talk at Waseda University

**Author(s) :** Ian Tobasco (University of Illinois Chicago)

**Abstract :** Kirigami metamaterials combine elasticity and geometry to create unusual bulk deformations. We derive a partial differential equation (PDE) for periodic kirigami, along with a strain-gradient like homogenized energy. Minimizing this energy amongst PDE solutions predicts the kirigami's deformation, as we demonstrate via experiments and simulations. Time permitting, we present analogous results for origami. A key step in our analysis is a rigidity inequality showing that the metamaterial's deformation is approximated by local mechanism motions.

## [03863] The macroscopic behavior of the Kagome lattice metamaterial

**Format :** Talk at Waseda University

**Author(s) :** Xuenan Li (New York University)

**Abstract :** Mechanism-based metamaterials are synthetic materials that exhibit microscale buckling in response to mechanical deformation. These artificial materials are like elastic composites, but more degenerate, since they can deform with zero elastic energy. We call such deformations with zero elastic energy mechanisms. My research focuses mainly on a rich example, the Kagome lattice metamaterial. This particular material has a huge variety of mechanisms, which might seem incompatible with having a meaningful macroscopic energy at first sight. In this talk, I will discuss the large-scale behavior of the kagome lattice metamaterial as a nonlinear homogenization problem and present our analysis of the well-defined macroscopic energy on this highly degenerate metamaterial. Our macroscopic theory reveals that compressive conformal maps achieve zero effective energy. I will also discuss the adequacy of our macroscopic theory with various numerical experiments. The theory is joint work with Robert Kohn, and the numerical results are joint work with Katia Bertoldi and Bolei Deng.

## [04196] Rayleigh waves in 2D extremal materials

**Format :** Online Talk on Zoom

**Author(s) :** Gengkai Hu (School of Aerospace Engineering, Beijing Institute of Technology)Yu Wei (School of Aerospace Engineering, Beijing Institute of Technology)

**Abstract :** Rayleigh waves are guaranteed in Cauchy materials with positive definite elasticity tensors. However it's proved that 2D extremal materials with Rank-deficient elasticity tensors cannot support Rayleigh waves, they can appear if the second gradient effect is considered. Microstructural models corresponding to the examined continuum models of Cauchy and second gradient elasticity are constructed, both continuum and discrete models agree very well in terms of the velocity and ellipticity for the predicted Rayleigh waves.

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00778 (2/3) : 5B @G801 [Chair: Anthony Stefan]

## [04081] Large-scale metasurface design with fast direct solvers

**Format :** Talk at Waseda University

**Author(s) :** Owen Miller (Yale University)

**Abstract :** Metasurfaces offer nanophotonic performance for centimeter-scale optics applications. Yet simulating such large structures is beyond current simulation capabilities. We demonstrate a 2D "fast direct" integral-equation solver that can simulate and design a high-efficiency, high-numerical-aperture metalens that is 20,000 wavelengths in diameter. For a visible wavelength of 500nm, this corresponds to a design diameter of 1cm, achieved with full simulations of Maxwell's equations.

## [04889] Relaxation of variational principles for bounding the effective operators of composites

**Format :** Talk at Waseda University

**Author(s) :** Aaron Welters (Florida Institute of Technology)

**Abstract :** An approach to the theory of composites is presented that allows a relaxation of the direct and dual minimization principles used to bound effective operators. This is based on representing the effective operator as the Schur complement of a positive semidefinite operator on a Hilbert space having a Hodge decomposition. We show the theory also applies in electric circuit theory for the Dirichlet-to-Neumann map and for the classical effective conductivity on a finite linear graph.

## [04890] Bessmertnyi realizations of effective tensors for metamaterial synthesis: conjectures and counterexamples

**Format :** Talk at Waseda University

**Author(s) :** Anthony Dean Stefan (Florida Institute of Technology)

**Abstract :** Effective tensors of isotropic n-phase composites are known to be homogeneous multivariate Herglotz functions. Recently, M. Bessmertnyi claimed to characterize any such rational function as being in the Bessmertnyi class because each partial Wronskian associated with it has a polynomial sum-of-squares representation. We disprove this claim by providing a counterexample derived from the basis generating polynomial for the Vámos matroid and give a conjecture on the realizability of effective tensors. Joint work with Aaron Welters.

00778 (3/3) : 5C @G801 [Chair: Maxence Cassier]

## [05015] Time domain analysis of resonant plasmonic nano-particles

**Format :** Talk at Waseda University

**Author(s) :** Pierre Millien (CNRS)Alice L. Vanel (CERN)Lorenzo Baldassari (RICE)Habib Ammari (ETHZ)

**Abstract :** We study the possible expansion of the electromagnetic field scattered by a strictly convex metallic nanoparticle with dispersive material parameters placed in a homogeneous medium in a low-frequency regime as a sum of modes oscillating at complex frequencies (diverging at infinity), known in the physics literature as the quasi-normal modes expansion. We show that such an expansion is valid in the static regime and that we can approximate the electric field with a finite number of modes. We then use perturbative spectral theory to show the existence, in a certain regime, of plasmonic resonances as poles of the resolvent for Maxwell's equations with non-zero frequency. We show that, in the time domain, the electric field can be written as a sum of modes oscillating at complex frequencies. We introduce renormalised quantities that do not diverge exponentially at infinity.

## [05234] Active exterior thermal cloaking

**Format :** Talk at Waseda University

**Author(s) :** Trent DeGiovanni (University of Utah)Fernando Guevara Vasquez (University of Utah)Maxence Cassier (CNRS, Institut Fresnel)Sébastien Guenneau (Imperial College London)

**Abstract :** We consider the problem of concealing an object, in the presence of a known probing fielding, from the perspective of thermal measurements. This is achieved using specially designed sources. Such a cloak can be constructed by using the Green identities; however, this requires a continuous strip of sources that encloses the object. In this talk, we demonstrate an alternative approach to this cloaking problem that uses only a few sources.

## [04994] Imaging conductivity with thermal noise induced currents

**Format :** Online Talk on Zoom

**Author(s) :** Fernando Guevara Vasquez (University of Utah)Trent DeGiovanni (University of Utah)

**Abstract :** Thermal fluctuations of charge carriers in a conductive body create small but detectable currents. We show that the variance of such currents can be used to image the conductivity of a body, including for complex conductivities. This is done by relating the stochastic problem to a deterministic inverse problem that is close to one arising in acousto-electric tomography.

# [00779] Advances in numerical methods for evolutionary PDEs and applications

**Session Time & Room :**

00779 (1/3) : 1C (Aug.21, 13:20-15:00) @A511

00779 (2/3) : 1D (Aug.21, 15:30-17:10) @A511

00779 (3/3) : 1E (Aug.21, 17:40-19:20) @A511

**Type :** Proposal of Minisymposium

**Abstract :** Several models in science, physics and engineering, are described by evolutionary systems of partial differential equations (PDEs). The purpose of the MS is to gather researcher interested in the development of innovative techniques for the numerical solution of a wide class of evolutionary problems, in several contexts: kinetic theory of rarefied gases, linear and nonlinear waves, viscoelasticity, multiphase flows, radiation hydrodynamics, traffic flows, shallow water, just to mention some examples. The mini-symposium will deal with several issues related to the numerical solution of such equations, including, among others, multi-scale issues, asymptotic preserving schemes, high order discretization in space and time, and stability analysis.

**Organizer(s) :** Sebastiano Boscarino, Giuseppe Izzo, Giovanni Russo

**Classification :** 65M06, 65M08, 65M12, 65M20, 65M22

**Minisymposium Program :**

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00779 (1/3) : 1C @A511 [Chair: Sebastiano Boscarino]

## [05243] Implicit-explicit time integration for thermal radiative transfer and radiation hydrodynamics

**Format :** Talk at Waseda University

**Author(s) :** Ben Scott Southworth (Los Alamos National Laboratory)

**Abstract :** Thermal radiative transfer (TRT) is an extremely stiff high-dimensional partial-integro-differential equation, which requires partitioned integration when coupled to hydrodynamics. I introduce an approximation of TRT that captures both stiff asymptotic limits, and IMEX framework requiring only one transport-sweep per timestep. I then discuss nonlinear coupling to hydrodynamics, which is complicated via equation-of-state relations. We derive a temperature closure and framework for semi-implicit-explicit integration of radiation hydrodynamics, demonstrating excellent convergence on stiff radiative shock problems.

## [03444] Semi-implicit numerical methods for level set equations

**Format :** Talk at Waseda University

**Author(s) :** Nikola Gajdošová (Slovak University of Technology in Bratislava)Katarína Lacková (Slovak University of Technology in Bratislava)Peter Frolkovič (Slovak University of Technology in Bratislava)

**Abstract :** We present semi-implicit higher order numerical methods to solve nonlinear level set equations for evolving interfaces. We introduce up to third order accurate unconditionally stable numerical schemes to solve advection by external velocity and speed in normal direction, and, eventually, regularized by a small curvature term. The methods have fully upwinded stencil in its implicit part so efficient algebraic solvers like fast sweeping methods can be applied.

## [05021] Efficient implicit methods for the Euler equations in Lagrangian coordinates

**Format :** Talk at Waseda University

**Author(s) :** Simone Chiocchetti (University of Stuttgart)Giovanni Russo (University of Catania)Sebastiano Boscarino (University of Catania)

**Abstract :** In this talk, we introduce a novel implicit numerical scheme for the multimaterial Euler equations in Lagrangian coordinates. The method takes advantage of the remarkable structure of the governing equations in Lagrangian coordinates, which admits a single scalar wave equation for the pressure field, generating a symmetric positive definite system of linear equations. At the same time, contacts are resolved exactly, due to the Lagrangian nature of the method, even without a Riemann solver.

## [03910] High-order semi-implicit schemes for evolutionary partial differential equations with higher order derivatives

**Format :** Talk at Waseda University

**Author(s) :** Sebastiano Boscarino (University of Catania, Italy)

**Abstract :** The aim of this work is to apply a semi-implicit (SI) strategy in an implicit-explicit (IMEX) Runge-Kutta (RK) setting introduced in (S. Boscarino- F. Filbet, G. Russo, JSC 2016) to a sequence of 1D time-dependent partial differential equations (PDEs) with high order spatial derivatives. This strategy gives a great flexibility to treat these equations, and allows the construction of simple linearly implicit schemes without any Newton's iteration. Furthermore, the SI IMEX- RK schemes so designed does not need any severe time step restriction that usually one has using explicit methods for the stability, i.e.  $\Delta t = O(\Delta t^k)$  for the k-th ( $k \geq 2$ ) order PDEs. For the space discretization, this strategy is combined with finite difference schemes. We illustrate the effectiveness of the schemes with many applications to dissipative, dispersive and biharmonic-type equations. Numerical experiments show that the proposed schemes are stable and can achieve optimal orders of accuracy.

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00779 (2/3) : 1D @A511 [Chair: Sebastiano Boscarino]

## [05310] Carbuncle-free, well-balanced, positivity preserving methods for the shallow water equations, with application to the circular hydraulic jump

**Format :** Talk at Waseda University

**Author(s) :** David I Ketcheson (King Abdullah University of Science and Technology)

**Abstract :** When a jet of fluid hits a flat plate, the resulting flow consists of two regimes separated by a hydraulic jump. We investigate the behavior of the jump for the shallow water equations. Numerical solvers tend to either exhibit artificial numerical instabilities or suppress the chaotic behavior at high Froude numbers. We propose a new entropy-based Riemann solver that is capable of avoiding carbuncles while allowing the fluid instability to manifest itself.

## [04458] New highly stiff-stable schemes for linear and nonlinear parabolic equations

**Format :** Talk at Waseda University

**Author(s) :** JIE SHEN (Purdue University)

**Abstract :** We construct a class of new highly stiff-stable schemes for linear and nonlinear parabolic equations based on Taylor expansions at time  $t_{n+k}$  where  $k \geq 1$  is a tunable parameter. We show that their numerical solutions are bounded unconditionally (resp. for sufficiently small time steps) for linear (resp. nonlinear) parabolic equations, and derive their optimal error estimates for a large class of nonlinear parabolic equations. We also present numerical results to show the advantages of the new schemes compared with the classic IMEX schemes based on Taylor expansions at time  $t_{n+1}$ .

## [05011] Finite-differences scheme for a tensor PDE model of bionetwork formation and applications

**Format :** Talk at Waseda University

**Author(s) :** Clarissa Astuto Giovanni Russo (University of Catania)Peter Markowich (King Abdullah University of Science and Technology)Daniele Boffi (KAUST)Jan Haskovec (KAUST)

**Abstract :** We propose a numerical method for the resolution of a complex biological network. We refer to the Cai-Hu model, where they hypothesized that the topology of the leaf pattern is governed by an optimization of the global energy consumption. The evolution in time of the fluid is governed by an elliptic-parabolic system of partial differential equations and we explore the resulting graph, showing important structural differences when changing the parameters.

## [04882] Asymptotic preserving scheme for ExB drift

**Format :** Talk at Waseda University

**Author(s) :** Umberto Zerbinati (University of Oxford)Giovanni Russo (University of Catania)

**Abstract :** In this talk, we explore an asymptotic preserving scheme for ExB drift. The key idea behind the scheme here presented is to treat the highly oscillatory component of the velocity using an exponential integrator. We will

apply this numerical scheme to particles in cell plasma simulation under the effect of a strong constant magnetic field.

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00779 (3/3) : 1E @A511 [Chair: Sebastiano Boscarino]

## [03846] Efficient simulation of high-dimensional kinetic equation

**Format :** Talk at Waseda University

**Author(s) :** Lukas Einkemmer (University of Innsbruck)

**Abstract :** Solving high-dimensional kinetic equations (such as the Vlasov equation or the Boltzmann equations) numerically is extremely challenging. Methods that discretize phase space suffer from the exponential growth of the number of degrees of freedom, the so-called curse of dimensionality, while Monte Carlo methods converge slowly and suffer from numerical noise. In addition, standard complexity reduction techniques (such as sparse grids) usually perform rather poorly due to the lack of smoothness for such problems. Dynamical low-rank techniques approximate the dynamics by a set of lower-dimensional objects. For those low-rank factors, partial differential equations are derived that can then be solved numerically. We will show that such dynamical low-rank approximations work well for a range of kinetic equations due to their capacity to handle non-smooth solutions and the fact that in many situations important physical limit regimes are represented very efficiently by such an approximation (e.g. fluid or diffusive limits).

## [04978] A conservative semi-Lagrangian method for inhomogeneous Boltzmann equation

**Format :** Talk at Waseda University

**Author(s) :** Seung Yeon Cho (Gyeongsang National University)Sebastiano Boscarino (University of Catania)Giovanni Russo (University of Catania)

**Abstract :** In this work, we propose a conservative semi-Lagrangian method for the Boltzmann equation. Semi-Lagrangian approach enables us to avoid CFL-type restrictions on the time step. High order in time is obtained by Runge-Kutta or Adams-Bashforth methods. High order in space is obtained by a high order conservative reconstruction which also prevents spurious oscillations. The fast spectral method with L2-correction guarantees spectral accuracy and conservation. Numerical results confirm the accuracy and efficiency of the methods.

## [03164] Asymptotic preserving and uniformly unconditionally stable schemes for kinetic transport equations

**Format :** Talk at Waseda University

**Author(s) :** Guoliang Zhang ( Shanghai Jiaotong University)

**Abstract :** In this talk, we will give uniformly unconditionally stable finite difference schemes for kinetic transport equations in the diffusive scaling. The schemes are based on a coupling of macroscopic and microscopic equations, by utilizing a backward semi-Lagrangian approach for transport part, and implicit method for the diffusive part. The schemes can be shown to be asymptotic preserving in the diffusive limit. Uniformly unconditional stabilities are verified by Fourier analysis. Numerical experiments will demonstrate their good performances.

## [04700] High order structure preserving schemes for MHD flows in all sonic Mach numbers

**Format :** Talk at Waseda University

**Author(s) :** Tao Xiong (Xiamen University)

**Abstract :** In this work, a high-order semi-implicit (SI) asymptotic preserving (AP) and divergence-free finite difference weighted essentially nonoscillatory (WENO) scheme is proposed for magnetohydrodynamic (MHD) equations. We consider the sonic Mach number  $\varepsilon$  ranging from 0 to  $\mathcal{O}(1)$ . High-order accuracy in time is obtained by SI implicit-explicit Runge-Kutta (IMEX-RK) time discretization. High-order accuracy in space is achieved by finite difference WENO schemes with characteristic-wise reconstructions. A constrained transport method is applied to maintain a discrete divergence-free condition. We formally prove that the scheme is AP. Asymptotic accuracy (AA) in the incompressible MHD limit is obtained if the implicit part of the SI IMEX-RK scheme is stiffly accurate. Numerical experiments are provided to validate the AP, AA, and divergence-free properties of our proposed approach. Besides, the scheme can well capture discontinuities such as shocks in an essentially non-oscillatory fashion in the compressible regime, while it is also a good incompressible solver with uniform large-time step conditions in the low sonic Mach limit.

# [00781] Physical and Mathematical Research on Transport on Slippery Surfaces

## **Session Time & Room :**

00781 (1/3) : 3D (Aug.23, 15:30-17:10) @D401

00781 (2/3) : 3E (Aug.23, 17:40-19:20) @D401

00781 (3/3) : 4C (Aug.24, 13:20-15:00) @D401

## **Type :** Proposal of Minisymposium

**Abstract :** In the past two decades numerous laboratories have microfabricated surfaces with the chemical and textural properties to mimic slippery surfaces found in nature, e.g. the superhydrophobic lotus leaf. This has been made possible by the continuing advances in nano/micro fabrication technology. This 3-part minisymposium will bring together engineers, physicists, and applied mathematicians in a multi-physics framework to discuss recent modelling and experimental applications.

**Organizer(s) :** Toby Kirk, Darren Crowdy

**Classification :** 76D07, 76D45, 76D55

## **Minisymposium Program :**

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00781 (1/3) : 3D @D401 [Chair: Toby Kirk]

## [03772] Flows through slippery tubes and annuli

### **Format :** Talk at Waseda University

**Author(s) :** Sebastian Zimmermann (RPTU Kaiserslautern-Landau)Clarissa Schönecker (RPTU Kaiserslautern-Landau)

**Abstract :** We present analytical models for the flow through tubes and annuli that possess slippery longitudinal slits along their surface. Firstly, these expressions can be employed with an arbitrary local slip length or shear stress being predefined at the slits, corresponding to an arbitrary Newtonian fluid. Secondly, the two solutions for tubes and annuli can be combined such that there is one fluid in the tube and another one in the annulus surrounding the tube.

## [03964] Numerical study of longitudinal flow over liquid infused surfaces

### **Format :** Talk at Waseda University

**Author(s) :** Hiroyuki Miyoshi (Imperial College London)Darren G. Crowdy (Imperial College London)

**Abstract :** A numerical method for the computation of two-phase pressure-driven longitudinal flow over liquid-infused surfaces is presented. These surfaces feature a periodic array of circular surface-embedded grooves filled with a subphase fluid that can enhance slip of an upper fluid, of different viscosity, flowing over it. A novelty of the numerical approach is that it deploys techniques from conformal geometry and complex analysis.

## [02965] Viscoplastic Flows through Grooved Superhydrophobic Channels

### **Format :** Talk at Waseda University

**Author(s) :** Seyed Mohammad Taghavi (Université Laval)Hossein Rahmani (Université Laval)

**Abstract :** We study the transport of viscoplastic fluids through channels with grooved superhydrophobic walls. To this end, we employ a comprehensive modeling approach and high-resolution numerical simulations and, in particular, consider longitudinal, transverse, and oblique orientations of the grooves. We use the perturbation theory to derive semi-analytical and closed-form solutions for the velocity fields, whose results are validated against our numerical simulations. Finally, we highlight the strong nonlinear effect of viscoplastic rheology and analyze the stabilizing/destabilizing effects of slip conditions on the flow.

## [04260] Jeffery's paradox for the rotation of a single 'stick-slip' cylinder

**Format :** Talk at Waseda University

**Author(s) :** Michael S Siegel (New Jersey Institute of Technology)Ehud Yariv (Technion)

**Abstract :** The two-dimensional fluid velocity due to the rotation of a superhydrophobic or 'stick-slip' cylinder in Stokes flow is

determined. We find that in the general case of an aperiodic distribution of stick and slip boundaries there is no solution in which the fluid velocity vanishes at infinity. This is the first example of Jeffery's paradox, typically associated with the flow due to the counter-rotation of two rigid cylinders, for a single cylinder.

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00781 (2/3) : 3E @D401 [Chair: Darren Crowdy]

## [03147] Experimental Applications of Slippery Liquid and Liquid-like-Solid Surfaces

**Format :** Talk at Waseda University

**Author(s) :** Glen McHale (The University of Edinburgh)Gary George Wells (The University of Edinburgh)Rodrigo Ledesma-Aguilar (The University of Edinburgh)

**Abstract :** The liquid Amontons' laws relate drop friction along a surface to the normal component of the capillary force. Here I outline work on low pinning surfaces which minimize the coefficient of static liquid friction. Using a liquid version of Young's law, I show low friction uni-directional and bi-directional droplet motion on liquid-infused surfaces. I also show surfaces with liquid-like solid coatings which overcome the risk of lubricant depletion and provide excellent anti-biofilm properties.

## [03590] Drop movement on lubricant-impregnated random textures

**Format :** Talk at Waseda University

**Author(s) :** Ratan Bharat Ahuja (Indian Institute of Technology Bombay)Amit Agrawal (Indian Institute of Technology Bombay)Suhas S Joshi (Indian Institute of Technology Indore)

**Abstract :** Lubricant-impregnated surfaces (LIS), owing to their omniphobicity have shown remarkable success against Newtonian, non-Newtonian and yield stress fluids. These surfaces are, however, prone to failure due to lubricant drainage. In this work, we fabricate random textures using the micro-EDM process in an attempt to prolong lubricant retention within grooves. Drop motion and velocity against lubricant of three different viscosities are captured using digital imaging. The results would aid in designing a robust LIS system.

## [05601] Asymptotic solutions for convection in longitudinal-fin heat sinks

**Format :** Talk at Waseda University

**Author(s) :** Toby Kirk (Imperial College London)Marc Hodes (Tufts University)

**Abstract :** We consider forced convection in a longitudinal-fin heat sink, i.e. a periodic array of thin, thermally conducting fins aligned with the direction of air flow. Sparrow, Baliga and Patankar (1978) solved this problem numerically, investigating the effect of the gap between the fin tips and the shroud. We solve the same problem in the realistic asymptotic limit of small fin spacing, and make connections to similar mathematical problems for liquid flow over superhydrophobic grooved surfaces.

## [02837] Inertial effects on the flow resistance of axial-groove heat pipes

**Format :** Talk at Waseda University

**Author(s) :** Haotian Jia (Tufts University)Marc Hodes (Tufts University)Toby Kirk (Imperial College London)

**Abstract :** We captured the effects of slowly-varying meniscus curvature on the flow resistance of the adiabatic section of an axial-groove heat pipe in the presence of inertial effects due to the changes in the cross-sectional areas of the liquid and vapor phases along the adiabatic section. This was done by extending a hybrid analytical-numerical method for a single-phase problem with slowly-varying meniscus curvature to two-phase.

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00781 (3/3) : 4C @D401 [Chair: Marc Hodes]

## [04287] Laminar drag reduction in surfactant-contaminated superhydrophobic channels

**Format :** Talk at Waseda University

**Author(s) :** Samuel Tomlinson (University of Manchester)Frédéric Gibou (University of California, Santa Barbara)Paolo Luzzatto-Fegiz (University of California, Santa Barbara)Fernando Temprano-Coleto (Princeton University)Oliver Jensen (University of Manchester)Julien Landel (University of Manchester)

**Abstract :** Although superhydrophobic surfaces (SHSs) show promise for drag reduction (DR) applications, their performance can be compromised by traces of surfactant. This question is addressed for a three-dimensional laminar flow in a periodic channel with SHSs along both walls, in the presence of soluble surfactant. The system exhibits multiple regimes where asymptotic solutions can be constructed, which compare favourably with numerics. This analysis provides a guide for designing surfactant-contaminated SHSs to maximise the DR for applications.

## [04901] Hypermobilization of superhydrophobic microchannels using light

**Format :** Talk at Waseda University

**Author(s) :** Michael Mayer (Imperial College London)Marc Hodes (Tufts University)Xiaozhe Hu (Tufts University)James Adler (Tufts University)

**Abstract :** This talk seeks to reframe the role of superhydrophobic surfaces, transforming them from passive lubricants to sources of active flow control. Utilizing a new model for the transport of photosurfactants, chemicals that can reversibly switch between two different states under differing light wavelengths, we show that it is possible to use light to generate surface tension gradients across menisci on superhydrophobic surfaces large enough to pump stationary fluid or even “hypermobilize” pressure driven flow.

## [04001] Analysis of surface diffusion on steady "stagnant caps" of surfactant

**Format :** Talk at Waseda University

**Author(s) :** Anna Elizabeth Curran (Imperial College London)Darren Crowdy (Imperial College London)

**Abstract :** We present a detailed analytical study, based on complex variable methods, which examines the remobilizing effects of surface diffusion on the structure of steady "stagnant caps" on a surfactant-loaded interface between a viscous fluid and a constant pressure region. Both insoluble and soluble surfactants are considered. We demonstrate mathematically how, in the presence of a convergent flow, stagnant caps can immobilize interfaces leading to sharp edges which can then be smoothed out by surface diffusion.

## [04344] Slip flow enhanced by Marangoni Stresses at a superhydrophobic air-water interface

**Format :** Online Talk on Zoom

**Author(s) :** dong song (Northwestern Polytechnical University)Baowei Song (Northwestern Polytechnical University)guang pan (Northwestern Polytechnical University)

**Abstract :** Surfactant-induced Marangoni stress at an air-water interface would balance the shearing stress which causes the collapse of drag reduction of superhydrophobic surfaces, whereas few solutions have been proposed to overcome the adverse influence due to the difficulty in removing surfactant from water. In this work, we demonstrate that, by changing the orientation or shape of the air-water interface with respect to the bulk flow, the balance between Marangoni stress and shear stress can serve as a driving force of an apparent slip flow without the external input of surfactant. The theoretical model agrees well with the experiments.

## [00782] Recent Advances on Mimetic Difference Methods

**Session Time & Room :** 1C (Aug.21, 13:20-15:00) @E802

**Type :** Proposal of Minisymposium

**Abstract :** Mimetic Difference Schemes are based on Mimetic Difference Operators which are discrete analogs of the continuous first order invariant operators divergence, gradient and curl. They have been used for quite some time to solve effectively a wide range of partial differential equations. In this mini symposium we will present recent advances on mimetic methods including energy conservation, stability analysis and extension of stability region via Mollification techniques. Numerical examples will be presented to illustrate the effectiveness of the methods

**Organizer(s) :** Jose E. Castillo

**Classification :** 65Nxx

**Minisymposium Program :**

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00782 (1/1) : 1C @E802 [Chair: Jose E Castillo]

## [01714] Fourth-order Mimetic Differential Operators Applied to the Convection-Diffusion Equation: A matrix Stability Analysis

**Format :** Talk at Waseda University

**Author(s) :** Jorge VILLAMIZAR (Universidad Industrial de Santander/Universidad de Los Andes)Larry Mendoza (Universidad Central de Venezuela)Giovanni Calderon (Universidad Industrial de Santander)Otilio Rojas (Universidad Central de Venezuela)Jose E Castillo (Computational Science Research Center at San Diego State University)

**Abstract :** The convection-diffusion equation describes physical phenomena where particles or energy are transferred within a physical system due to the processes of diffusion and convection. In this work, we investigate discretization framework based on the mimetic fourth-order finite-difference staggered-grid Castillo-Grone (*CG*) operators, which has a sextuple of free parameters. We study the dependency of the stability and precision properties of our numerical scheme based on these CG free parameters, and propose parameters that favor both properties. We compare our results with CG parameters previously mentioned in the literature, including those leading to mimetic operators of minimum bandwidth.

## [01788] Discrete mollification results in mimetic difference schemes applied to the convection-diffusion-reaction equation

**Format :** Talk at Waseda University

**Author(s) :** Julio Cesar Carrillo-Escobar (Professor)Giovanni Ernesto Calderon-Silva (Universidad Industrial de Santander)

**Abstract :** It is usual to have stability restrictions when using either an explicit finite differences or a mimetic differences schemes, proposed by Castillo in 2003, to obtain numerical solutions for the convection-diffusion-reaction equation of an incompressible fluid with a source term. In this work, we analyze the effects, in precision and stability, when applying the discrete mollification proposed by Acosta in 2008 to these schemes in mimetic differences.

## [01936] Numerical Energy Conservation Mimetic Scheme For The Advection Equation

**Format :** Online Talk on Zoom

**Author(s) :** Anand Srinivasan (San Diego State University)Jose E Castillo (Computational Science Research Center at San Diego State University)

**Abstract :** The advection equation  $u_t + \nabla \cdot u = 0$  is a hyperbolic partial differential equation that conserves energy. The numerical solution of the advection equation obtained using the traditional finite difference methods often fails to discretely conserve this numerical energy. Mimetic finite difference methods are structure-preserving and are thus well-suited for hyperbolic problems such as the advection equation. The Mimetic methods of Castillo et al discretely mimic the extended Gauss' divergence theorem, and are therefore a faithful discretization of the continuum vector calculus identities. These methods work on a staggered spatial grid and achieve even order of accuracy at the boundaries as well as the interiors of the domain. The temporal discretization obtained from the Leapfrog scheme is staggered in time. The staggered Mimetic-Leapfrog scheme conserves the numerical energy for the advection equation. In this talk, we present the numerical results illustrating the energy-conserving property of the second order Mimetic-Leapfrog scheme. Stability results of the scheme are also presented.

## [01939] Energy Conservation for Mimetic Scheme for Advection Equation

**Format :** Talk at Waseda University

**Author(s) :** Jose E Castillo (Computational Science Research Center at San Diego State University)

**Abstract :** Mimetic difference schemes are based on discrete analogs of differential operators, gradient, divergence, and curl, that not only preserve their vector calculus identities but also hold discrete counterparts of integral formulas.

A proof of the energy conservation property of second-order mimetic difference schemes is presented for the one-dimensional advection PDE. This proof leverages on the discrete analog of the integration by parts mimetic difference property

# [00783] PDE Eigenvalue Problems: Computational Modeling and Numerical Analysis

**Session Time & Room :**

00783 (1/5) : 3C (Aug.23, 13:20-15:00) @G701

00783 (2/5) : 3D (Aug.23, 15:30-17:10) @G701

00783 (3/5) : 3E (Aug.23, 17:40-19:20) @G701

00783 (4/5) : 4C (Aug.24, 13:20-15:00) @G701

00783 (5/5) : 4D (Aug.24, 15:30-17:10) @G701

**Type :** Proposal of Minisymposium

**Abstract :** Eigenvalue problems of partial differential equations have many important applications in science and engineering, e.g., design of solar cells for clean energy, calculation of electronic structure in condensed matter, extraordinary optical transmission, non-destructive testing, photonic crystals, and biological sensing. This mini-symposium focuses on the computation modeling and numerical analysis for PDE eigenvalue problems. It intends to bring the leading researchers to discuss the recent developments and build collaborations among participants of various backgrounds.

**Organizer(s) :** Hengguang Li, Xuefeng Liu, Jeffrey Oval, Jiguang Sun

**Classification :** 35P30, 47A75, 65N25, 65H17, 65F18

**Minisymposium Program :**

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00783 (1/5) : 3C @G701 [Chair: Xuefeng Liu]

## [01926] Eigenvalues in Inverse Scattering

**Format :** Talk at Waseda University

**Author(s) :** Peter Monk (University of Delaware)

**Abstract :** Transmission eigenvalues can be determined from multistatic scattering data over a range of frequencies and have been suggested as target signatures in inverse scattering. To avoid the need for data over a range of frequencies other artificial eigenvalue problems can be derived by modifying the far field operator. We shall consider “modified transmission eigenvalues” for thin structures. Numerical results will show that a few eigenvalues of each type can be determined from multi-static scattering data.

## [01744] Inverse eigenvalue problems for inferring crystal structure from neutron scattering data

**Format :** Talk at Waseda University

**Author(s) :** Guannan Zhang (Oak Ridge National Laboratory)

**Abstract :** We are interested in inferring the atomic structure of crystal materials from neutron scattering data. The atomic structure is modeled by a parameterized Hamiltonian matrix and the measurements in neutron scattering experiments are the eigenvalues and functionals of the eigenvectors of the Hamiltonian matrix. The goal is to find

the optimal parameter in the Hamiltonian matrix to match the scattering data. The main challenge is that the spectrum of the Hamiltonian matrix is very sensitive to its parameters, which leads to a very rough loss landscape. To address this issue, we propose a new loss function that utilize the characteristic polynomial of the Hamiltonian matrix as the loss function. When a matrix has the same eigenvalues as the measurement data, the characteristic loss is zero. Our experiments show that the new loss has a much smoother landscape for an optimization algorithm to find a satisfactory solution. We have demonstrated the effectiveness of our approach in solving the crystal field parameters from neutron scattering data.

## [01689] Application of Prolate Eigensystem to Born Inverse Scattering

**Format :** Talk at Waseda University

**Author(s) :** Shixu Meng (Academy of Mathematics and Systems Science, Chinese Academy of Sciences)

**Abstract :** This talk discusses the application of generalized prolate spheroidal wave functions and eigenvalues (in short prolate eigensystem) to Born inverse scattering problems. We first establish a Picard criterion to reconstruct the contrast. Further motivated by a Sturm-Liouville theory associated with the prolate eigensystem, we give a spectral cutoff regularization for noisy data and an explicit stability estimate for contrast in  $H^s$ , \$0

## [01864] Computational tools for exploring eigenvector localization

**Format :** Talk at Waseda University

**Author(s) :** Jeffrey Ovall (Portland State University)Robyn Reid (Portland State University)

**Abstract :** It is well-known that waves can often be decomposed as an infinite sum where each term in the sum is a product of a function varying only in time and a function varying only in space. The spatial functions are often called standing waves in this context, and are eigenvectors of a spatial differential operator associated with the medium through which the waves are propagating.

It is not as well-known that properties of the medium can cause some eigenvectors to be strongly spatially localized.

A practical consequence of eigenvector localization is that waves at certain frequencies can be trapped'' at some location or channelled'' along some favorable path. Such features are of interest in the design of structures having desired acoustic or electromagnetic properties: sound-mitigating outdoor barriers and next generation organic LEDs and solar cells are examples of this design principle in action. There remain many open problems related to understanding and exploiting this kind of localization, and we will discuss a computational approach that we expect will provide useful insight. More specifically, we focus on the issue of eigenvector localization, outlining our computational approach and providing theoretical, heuristic, and empirical support for it through several examples (with many pictures).

00783 (2/5) : 3D @G701 [Chair: Jeffrey Ovall]

## [01877] LOWER EIGENVALUE BOUNDS FOR THE HARMONIC AND BI-HARMONIC OPERATOR

**Format :** Talk at Waseda University

**Author(s) :** Carsten Carstensen (Humboldt-Universitaet zu Berlin umboldt-Universitaet zu Berlin)Sophie Puttkammer (Humboldt-Universitaet zu Berlin umboldt-Universitaet zu Berlin)

**Abstract :** Like guaranteed upper eigenvalue bounds with conforming finite element methods, guaranteed lower eigenvalue bounds (GLB) follow from min-max principles. Part 1 recalls GLB for the simplest second-order and fourth-order eigenvalue problems from a simple post-processing. The maximal mesh-size therein destroys nice adaptive mesh-refining and motivates a new methodology. Part 2 presents a new method with fine-tuned stabilization for the direct computation of GLB. Part 3 studies an optimal adaptive mesh-refining algorithm.

## [01904] Reduced order models for parametric PDE eigenvalue problems

**Format :** Talk at Waseda University

**Author(s) :** Daniele Boffi (KAUST)

**Abstract :** It is well known that the approximation of parametric eigenvalue problems offer much more challenges than the corresponding source problems. This is due in particular to the lack of smoothness of the solutions with respect to the parameters. Multiplicities, clusters, and crossing of eigenvalues must be dealt with in an appropriate way in order achieve meaningful and accurate solutions.

We discuss how to track the eigensolutions in presence of multidimensional parameters and we propose new ideas for the model order reduction of eigenvalues problems.

## [01686] Verification of guaranteed lower eigenvalue bounds form a hybrid-high order method

**Format :** Talk at Waseda University

**Author(s) :** Carsten Carstensen (Humboldt-Universität zu Berlin)Benedikt Gräßle (Humboldt-Universität zu Berlin)Ngoc Tien Tran (Friedrich-Schiller-Universität Jena)

**Abstract :** A new class of skeletal methods provides direct guaranteed lower eigenvalue bounds (GLB) under verifiable assumptions on the maximal mesh-size and discretisation parameters.

The verification of the GLB condition requires the knowledge of some stability constants and its validity implies that the computed discrete eigenvalue is already a GLB. This talk discusses the explicit estimation of the stability constants for the hybrid-high order (HHO) eigenvalue solver of Carstensen-Ern-Puttkammer [Numer.Math. 149, 2021] and its recent modification with an even simpler p-robust parameter selection.

We prove an a priori quasi-best approximation property and establish stabilization-free reliable and efficient a posteriori error control. Computer benchmarks provide striking numerical evidence for optimal high-order convergence rates of the associated adaptive mesh-refining algorithm.

## [01859] Poisson solvers for the biharmonic eigenvalue problem with the Navier boundary condition

**Format :** Talk at Waseda University

**Author(s) :** Baiju Zhang (Beijing Computational Science Research Center )Hengguang Li (Wayne State University)Zhimin Zhang (Wayne State University)

**Abstract :** Consider the biharmonic eigenvalue problem with the Navier boundary condition. The Ciarlet-Raviart mixed method solves this problem by decomposing the 4th-order operator into two Laplacians but can produce spurious eigenvalues in non-convex domains. To overcome this difficulty, we adopt a recently developed mixed method, which decomposes the biharmonic equation into three Poisson equations and still recovers the original solution. Using this idea, we design an efficient biharmonic eigenvalue algorithm, which contains only Poisson solvers. With this approach, eigenfunctions can be confined in the correct space and thereby spurious modes in non-convex domains are avoided. Numerical results will be reported to validate the algorithm.

00783 (3/5) : 3E @G701 [Chair: Hengguang Li]

## [01910] Why Spectral Methods are preferred in PDE Eigenvalue Problems?

**Format :** Talk at Waseda University

**Author(s) :** Zhimin Zhang (CSRC & WSU)

**Abstract :** When approximating PDE eigenvalue problems by numerical methods such as finite difference and finite element, it is common knowledge that only a small portion of numerical eigenvalues are reliable. As a comparison, spectral methods may perform extremely well in some situation, especially for 1-D problems. In addition, we demonstrate that spectral methods can outperform traditional methods and the state-of-the-art method in 2-D problems even with singularities.

## [01726] High-precision guaranteed eigenvalue bounds using higher order finite elements and graded meshes

**Format :** Talk at Waseda University

**Author(s) :** Xuefeng LIU (Niigata University)

**Abstract :** The projection residue error-based eigenvalue bound proposed by the author has a drawback that it is influenced by the worst-case projection error and is not able to take the advantage of non-uniform meshes such as

graded meshes. To address these issues, we propose a new method based on the Kato-Lehmann-Goerisch theorem to obtain high-precision eigenvalue bounds that take full advantage of higher-order FEMs, graded meshes, and possible strong regularities of eigenfunctions.

## [01925] Comparison of guaranteed lower eigenvalue bounds with three skeletal methods

**Format :** Talk at Waseda University

**Author(s) :** Emilie Pirch (Friedrich-Schiller-Universität Jena) Carsten Carstensen (Humboldt-Universitaet zu Berlin) Benedikt Gräßle (Humboldt-Universität zu Berlin)

**Abstract :** The focus of this talk is the comparison of three specially tailored skeletal hybrid schemes which provide direct guaranteed lower eigenvalue bounds (GLB) for the Dirichlet eigenvalue problem of the Laplacian. While the scheme presented in (Carstensen-Zhai-Zhang2020) has established the groundwork with a first formulation of the conditions under which GLB can be computed with a hybridized discontinuous Galerkin (HDG) method, a further development in (Carstensen-Ern-Puttkammer2021) results in a modified hybrid-high order method with a simplified stabilization term. However, it involves two parameters whose choice can be unclear due to stability estimates with constants which depend on the polynomial degree  $p$  of the approximation spaces and numerical computations show a lack of robustness. (Carstensen-Gräßle-Tran2022,subm.) presents a different stabilization which uses a  $p$ -robust parameter. Numerical examples for all three methods and various polynomial degrees with optimal orders of convergence will be shown in this talk. The details of the qualitative differences in the computation of GLB and possible further practical improvements will be discussed.

## [02081] Novel spectral methods using multivariate Muntz polynomials/functions for Schrodinger eigenvalue problems with singular potentials

**Format :** Talk at Waseda University

**Author(s) :** Huiyuan Li (Institute of Software Chinese Academy of Sciences)

**Abstract :** In this talk, we first introduce multivariate Muntz ball polynomials and Muntz Hermite functions, and then propose novel spectral methods for solving the eigenvalue problems of the Schrodinger operators  $[-\Delta + c/|x|^2] + z|x|^{q/p}$  and  $-\nabla \cdot (|x|^{2\mu} \nabla) + c|x|^{2\mu-2}$ . The Muntz polynomials/functions are tailored to fit the singularities of the eigenfunctions and are orthogonal with respect to the inner product associated with the underlying Schrodinger operator. Numerical experiments demonstrate the efficiency and the exponential order of convergence of our methods, and validate the superiority over other methods.

00783 (4/5) : 4C @G701 [Chair: Xuefeng Liu]

## [02157] Continuity and differentiability of eigenvalues of Laplacian with respect to general domain perturbations

**Format :** Talk at Waseda University

**Author(s) :** Takuya Tsuchiya (Ehime University)

**Abstract :** We consider the eigenvalue problems of Laplacian on bounded domains with Lipschitz boundaries. Suppose that a domain is smoothly perturbed, and the perturbation is parametrized in  $t$ .

In this talk, we discuss about continuity and differentiability of perturbed eigenvalues with respect to the parameter  $t$ .

## [01803] GPU-accelerated high order mimetic finite difference methods for Maxwell equations and eigenproblems

**Format :** Talk at Waseda University

**Author(s) :** Yan Xu (University of Science and Technology of China)

**Abstract :** In this paper, we consider the eigenvalue problem of the three-dimensional time-harmonic Maxwell equations. The problem is discretized by the general mimetic finite difference method (MFDM), which is based on  $L^2$  de Rham complex and has a deep relation with finite element exterior calculus theory. The discretization for the shifted differential operator is also covered. The main challenge arises from the large null space of the approximate curl operator. We introduce an auxiliary scheme to reach nontrivial eigenpairs without going through null space. We design a multigrid-type preconditioner for the algorithm to reduce the iteration count of the iterative eigensolver. Most of the algorithm are basic matrix and vector operators, which are fine-grained parallelism and

can be easily accelerated by GPU. Numerical examples of the band structures of three-dimensional photonic crystals are presented to demonstrate the capability and efficiency of the algorithm.

## [01881] Compatible Approximation of Holomorphic Eigenvalue Problems

**Format :** Online Talk on Zoom

**Author(s) :** Martin Halla (eorg-August Universität Göttingen, Institut für Numerische und Angewandte Mathematik)

**Abstract :** I consider Galerkin approximations of EVP for holomorphic operator functions, which arise e.g. from finite element discretizations of PDE eigenvalue problems. The convergence is ensured for "regular" approximations (Karma (1996)). This property is unconditionally satisfied for weakly coercive problems. However, for non weakly coercive problems there exist hardly any results. I present a technique to prove the regularity for such cases, which builds upon the weak T-coercivity of the continuous problem.

## [01914] The new computational method on elastic transmission eigenvalue problem

**Format :** Online Talk on Zoom

**Author(s) :** Yingxia Xi (Nanjing University of Science and Technology)Xia Ji (Beijing Institute of Technology)Shuo Zhang (Academy of Mathematics and Systems Science)

**Abstract :** We will present a finite element scheme for the elastic transmission eigenvalue problem written as a fourth order eigenvalue problem. The scheme uses piecewise cubic polynomials and obtains optimal convergence rate. Compared with other low-degree and nonconforming finite element schemes, the scheme inherits the continuous bilinear form which does not need extra stabilizations and is thus simple to implement.

00783 (5/5) : 4D @G701

## [00785] Learning Dynamical Systems by Preserving Symmetries, Energies, and Variational Principles

**Session Time & Room :**

00785 (1/2) : 5B (Aug.25, 10:40-12:20) @F308

00785 (2/2) : 5C (Aug.25, 13:20-15:00) @F308

**Type :** Proposal of Minisymposium

**Abstract :** Dynamical systems abound in engineering and science, and their accurate long-time simulation and outer-loop applications such as control, design and uncertainty quantification remains a computational challenge. From first principles modeling of physical systems, it is clear that many of these dynamical systems have a natural geometric structure (e.g., Hamiltonian, Lagrangian, metriplectic) or symmetry (translational, rotational). Exploiting and enforcing this structure in physics-based learning methods remains imperative for capturing the underlying physics accurately. This minisymposium highlights recent developments in physics-preserving learning for dynamical systems, such as: Lagrangian/Hamiltonian neural networks, sparse identification of nonlinear dynamics (SINDy), operator inference, preservation of conservation laws, the incorporation of interconnection and modular structure, structure-preserving system identification and other machine learning approaches.

**Organizer(s) :** Boris Kramer, Yuto Miyatake

**Classification :** 37Exx, 41-xx, 37Kxx, 37Kxx, 37Kxx

**Minisymposium Program :**

00785 (1/2) : 5B @F308 [Chair: Yuto Miyatake]

## [01395] Symplectic Model Reduction on Quadratic Manifolds

**Format :** Talk at Waseda University

**Author(s) :** Boris Kramer (University of California San Diego)

**Abstract :** When Hamiltonian models are used for long-term simulation, constraints on CPU hours need to be met. Structure-preserving model reduction for Hamiltonian systems addresses this computational issue by projecting Hamilton's equations of the full-order model onto linear symplectic subspaces, which can yield inaccurate results for problems with a slowly decaying Kolmogorov n-width. We present symplectic structure-preserving reduced-order modeling of Hamiltonian systems using quadratic manifolds. We demonstrate the proposed method on wave equations in 1-D and 2-D.

## [01373] Identification of variational principles, symmetries, and conservation laws from data

**Format :** Talk at Waseda University

**Author(s) :** Yana Lishkova (University of Oxford)Paul Scherer (University of Cambridge)Steffen Ridderbusch (University of Oxford)Mateja Jamnik (University of Cambridge)Pietro Lio (University of Cambridge)Sina Ober-Blöbaum (Paderborn University)Christian Offen (Paderborn University)

**Abstract :** The identification of equations of motions of dynamical systems from data as well as dynamical properties such as symmetries and conservation laws is an important task in the context of system identification. I will show a framework based on Lie group theory to learn a variational principle governing a dynamical system which can identify variational symmetries and conservation laws along the way. Identified symmetries prove helpful when the learned equations of motions are integrated numerically.

## [01597] Data-driven structure-preserving model reduction for stochastic Hamiltonian systems

**Format :** Talk at Waseda University

**Author(s) :** Tomasz Tyranowski (Max Planck Institute for Plasma Physics)

**Abstract :** In this work we demonstrate that SVD-based model reduction techniques known for ordinary differential equations, such as the proper orthogonal decomposition, can be extended to stochastic differential equations in order to reduce the computational cost arising from both the high dimension of the considered stochastic system and the large number of independent Monte Carlo runs. We also extend the proper symplectic decomposition method to stochastic Hamiltonian systems, both with and without external forcing, and argue that preserving the underlying symplectic or variational structures results in more accurate and stable solutions that conserve energy better than when the non-geometric approach is used. We validate our proposed techniques with numerical experiments for a semi-discretization of the stochastic nonlinear Schrödinger equation and the Kubo oscillator.

## [01793] Learning video models with Lagrangian/Hamiltonian neural networks

**Format :** Talk at Waseda University

**Author(s) :** Christine Allen-Blanchette (Princeton University)

**Abstract :** The dynamics underlying object and camera motion in a video typically evolve on a low-dimensional manifold with unknown structure and dimension. While prior work has used the Hamiltonian formalism to give a physically meaningful interpretation to this manifold, the problem of discovering the manifold structure and dimension remains unaddressed. We introduce a Hamiltonian neural network for video generation where the structure and dimension of the phase-space are implicitly learned from data. To achieve this we introduce a GAN-based video generation pipeline which embeds a learned transformation from a Gaussian distribution to the phase-space manifold, and captures the underlying dynamics of the video in a Hamiltonian neural network motion model.

## [02758] Structure-preserving exterior calculus for GNNs: surrogates, physics discovery, and causality

**Format :** Online Talk on Zoom

**Author(s) :** Nathaniel Trask (Sandia National Laboratories)

**Abstract :** We present a graph exterior calculus which may be used to design graph neural network which naturally preserve mathematical and physical structure without resorting to physics-informed regularizers. The calculus provides a framework for proving numerical stability, conservation, preservation of geometric symmetries, thermodynamic consistency, gauge conditions, and other properties more typical of traditional PDE discretization. In this setting we discover Whitney forms encoding physically relevant subdomains, their boundaries, and flux conservation laws for multiphysics/multiscale systems. We introduce ongoing applications work using this to discover structure-preserving surrogates which exhibit 100000x speedup for typical problems while guaranteeing mathematical robustness, and introduce recent extensions discovering causal relationships in scientific datasets.

## [00787] Space Weather: Modeling, Surrogates and Uncertainty Quantification

**Session Time & Room :** 5D (Aug.25, 15:30-17:10) @F308

**Type :** Proposal of Minisymposium

**Abstract :** Electronic technologies that govern modern life, such as the Global Positioning System, are dependent on satellite technologies, which require accurate space weather models with quantified uncertainties to operate safely and efficiently. Uncertainties in space weather models are wide-ranging. They can stem from how the models are driven, e.g., parameters, initial conditions, forcing, and from the treatment of the internal physics and numerics. For example, predictions of thermospheric density must account for model-form and parametric uncertainty in models of thermal conductivity and Nitric Oxide cooling. This minisymposium presents broad class of novel UQ methods for the exciting application of space weather.

**Organizer(s) :** Boris Kramer, Enrico Camporeale

**Classification :** 37Exx, 62Fxx, 62Gxx, 76Xxx

**Minisymposium Program :**

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00787 (1/1) : 5D @F308 [Chair: Boris Kramer]

## [02020] Model Calibration for Ensemble CME Simulation with the SWMF

**Format :** Talk at Waseda University

**Author(s) :** Hongfan Chen (University of Michigan)Yang Chen (University of Michigan)Xun Huan (University of Michigan)Bartholomeus van der Holst (University of Michigan)Shasha Zou (University of Michigan)Zhenguang Huang (University of Michigan) Nishtha Sachdeva (University of Michigan) Aniket Jivani (University of Michigan)Daniel Iong (University of Michigan)Ward Manchester (University of Michigan)Gabor Toth (University of Michigan)Yifu An (University of Michigan)

**Abstract :** The Space Weather Modeling Framework (*SWMF*) enables ensemble coronal mass ejection (*CME*) simulation based on coupled first principles and/or empirical models. The main challenge of calibrating unknown parameters of such physics-based models lies in high computational complexity and potential model inadequacy. In this talk, we present model calibration for the parameters of Gibson-Low flux-rope-based CMEs. Leveraging machine learning tools, we quantify the uncertainty in flux-rope parameters by assimilating in-situ and remote observations.

## [02101] Model reduction with data assimilation for thermospheric mass density forecasting

**Format :** Talk at Waseda University

**Author(s) :** Peng Mun Siew (Massachusetts Institute of Technology)Richard Linares (Massachusetts Institute of Technology)

**Abstract :** Earth atmospheric drag remains one of the main sources of uncertainties for orbit prediction of space objects residing in the Low Earth Orbit. In this work, we explore the usage of machine learning-based techniques to develop a data-driven dynamic reduced-order model for real-time forecasting of the thermospheric density field.

The high-dimensional thermospheric density field is projected onto a lower-dimensional latent space using nonlinear embedding via the deep encoder network.

## [01696] Bayesian Parameter Estimation for Ambient Solar Wind Models

**Format :** Online Talk on Zoom

**Author(s) :** Opal Issan (University of California San Diego)Boris Kramer (University of California San Diego)Enrico Camporeale (National Oceanic and Atmospheric Administration)

**Abstract :** The solar wind is an essential driver of space weather geomagnetic storms. A significant challenge in using first-principle solar wind models is estimating input parameters that can not be directly measured. Thus, we need to quantify the uncertainty of such input parameters on the solar wind. We perform global sensitivity analysis to understand which parameters influence the model output the most and learn the posterior distribution of the most influential input parameters via Bayesian inference.

## [02759] A multi-fidelity boosted method with built-in uncertainty quantification and its application to geomagnetic storms prediction

**Format :** Online Talk on Zoom

**Author(s) :** Andong Hu (CIRES, CU Boulder)Enrico camporeale (CIRES, CU Boulder)Brian swiger (CIRES, CU Boulder)

**Abstract :** An multi-fidelity based Gated Recurrent Unit (GRU) method is developed to assist ensemble technique to forecast extreme space weather events and their reliability. We have implemented this method on two space weather applications, i.e., 1) a one-to-six-hour lead-time model that predicts the value of Disturbance storm time (Dst) using solar wind (SW) data; and 2) an geoelectric field model with multi-hour leading time using SW and SuperMag data.

## [00789] Algorithmic advances in computational quantum mechanics

**Session Time & Room :**

00789 (1/3) : 3C (Aug.23, 13:20-15:00) @D405

00789 (2/3) : 3D (Aug.23, 15:30-17:10) @D405

00789 (3/3) : 3E (Aug.23, 17:40-19:20) @D405

**Type :** Proposal of Minisymposium

**Abstract :** Chemistry, physics, and materials science have benefited tremendously from advances in algorithmic tools for the simulation of quantum systems. In recent years, ideas developed in collaboration with the applied mathematics community have played an increasingly prominent role. This minisymposium will focus on recent algorithmic advances in computational quantum mechanics driven by numerical linear algebra, numerical methods for partial differential equations and integral equations, fast algorithms for the manipulation of structured operators, convex optimization, tensor networks, randomized algorithms, and machine learning methods.

**Organizer(s) :** Jason Kaye, Michael Lindsey

**Classification :** 81-08, 65Z05, Computational Quantum Physics

**Minisymposium Program :**

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00789 (1/3) : 3C @D405 [Chair: Jason Kaye]

## [04860] Deterministic algorithms for the efficient evaluation of Feynman diagrams

**Format :** Talk at Waseda University

**Author(s) :** Jason Kaye (Flatiron Institute, Simons Foundation)Denis Golež (Jožef Stefan Institute)Hugo U. R. Strand (Örebro University)

**Abstract :** The evaluation of Feynman diagrams is a fundamental computational task, and bottleneck, in Green's function methods for quantum many-body calculations. Mathematically, diagrammatic expressions take the form of high-dimensional integrals involving products of low-dimensional functions. Numerical methods for the part\_2

efficient evaluation of these diagrams are predominantly based on Monte Carlo or quasi-Monte Carlo sampling. I will discuss recent progress in algorithms which exploit the structure of the diagrammatic expressions to obtain efficient deterministic algorithms. In particular, I will describe an algorithm for the evaluation of imaginary time diagrams based on sum-of-exponentials representations of Green's functions, and mention a related algorithm based on the decomposition of integrands into tensor trains using cross interpolation.

## [04522] Quantics tensor trains meet quantum physics

**Format :** Talk at Waseda University

**Author(s) :** Hiroshi Shinaoka (Saitama University)

**Abstract :** In this talk, we apply quantics tensor train (QTT) to numerical simulations in quantum field theories<sup>1</sup>. Using QTT, we compress space-time dependence of correlation functions and solve equations in the compressed form. We also introduce quantics tensor cross interpolation to enhance the power of QTT-based calculations<sup>2</sup>. 1. H. Shinaoka et al., arXiv:2210.12984v2 (to appear in Phys. Rev. X), 2. M. K. Ritter et al., including H. Shinaoka, arXiv:2303.11819v2.

## [03608] Circuit Forms of Compressed Functions and Operators with Applications

**Format :** Talk at Waseda University

**Author(s) :** Edwin Miles Stoudenmire (Flatiron Institute)

**Abstract :** Recently there has been growing interest in representing functions as tensor networks using the "quantized tensor train" format, which enables algorithms (integration, function optimization, ...) typically scaling logarithmically in the grid size. I will discuss techniques to construct functions and operators in this format using non-unitary analogues of quantum circuits. This leads to fast algorithms for Fourier and wavelet transforms, and has promising applications for systems of continuous variables in classical and quantum physics.

## [05166] Tensor-network sketching and many-body physics

**Format :** Talk at Waseda University

**Author(s) :** Yuehaw Khoo (The University of Chicago)Yoonhaeng Hur (The University of Chicago)Yian Chen (The University of Chicago)Jeremy Hoskins (The University of Chicago)Michael Lindsey (UC Berkeley)Edwin Miles Stoudenmire (Flatiron Institute)

**Abstract :** We study how a function can be estimated as a low-rank tensor-network from Monte-Carlo samples, without the use of optimization and without the curse of dimensionality. We demonstrate the usefulness in generative modeling and many-body physics.

00789 (2/3) : 3D @D405 [Chair: Michael Lindsay]

## [03946] Analyzing Non-equilibrium Quantum Many-body Dynamics by Dynamic Mode Decomposition

**Format :** Talk at Waseda University

**Author(s) :** Chao Yang (Lawrence Berkeley National Lab)Jia Yin (Lawrence Berkeley National Lab)Yuanran Zhu (Lawrence Berkeley National Lab)

**Abstract :** A practical way to compute time-dependent observables of an out-of-equilibrium quantum many-body system is to focus on the single-particle Green's function defined on the Keldysh contour. The equation of motion satisfied by such a Green's function is a set of nonlinear integro-differential equations called the Kadanoff-Baym equations. We will describe numerical methods for solving these equations and show how to use dynamic mode decomposition to reduce their computational complexity.

## [05317] Some mathematical insights on DMET

**Format :** Talk at Waseda University

**Author(s) :** Fabian Maximilian Faulstich (Rensselaer Polytechnic Institute)

**Abstract :** High-accuracy methods are crucial for simulating static correlated systems, but they often scale severely. DMET can solve this by scaling highly accurate solvers. This talk shows that the exact ground-state density matrix is a fixed point of DMET for non-interacting systems, with a unique physical solution in the weakly-interacting regime. DMET is exact to first order in the coupling parameter, and numerical simulations confirm these results. Assumptions behind their validity are also discussed.

## [04977] Efficient algorithms for Brillouin zone and frequency integration

**Format :** Talk at Waseda University

**Author(s) :** Lorenzo Xavier Van Munoz (Massachusetts Institute of Technology)Jason Kaye (Flatiron Institute, Simons Foundation)Sophie Beck (Flatiron Institute, Simons Foundation)

**Abstract :** Brillouin zone integration is a standard operation in electronic structure calculations used to compute numerous physical observables. For integrands with broad features at scale  $\eta$ , standard equispaced integration methods are highly effective. However, when  $\eta$  is small, adaptive methods become necessary to achieve converged results. We extend these adaptive, high-order accurate methods to problems with an additional frequency integral, such as the optical conductivity, and discuss how to control the error in these iterated integrals.

## [04273] Extraction of resonant states in systems with defects

**Format :** Talk at Waseda University

**Author(s) :** Eloise Letournel (CERMICS)Antoine Levitt (Université Paris Saclay (LMO))Luigi Genovese (CEA Grenoble)Ivan Duchemin (CEA Grenoble)Simon Ruget (CERMICS)

**Abstract :** We introduce a numerical method to compute resonances induced by localized defects in crystals. We express the resonance in terms of a “resonance source” strictly localized within the defect region. We then compute a kernel equation, applying against this source the Green’s function of the perfect crystal, which we show can be computed efficiently by a complex deformation of the Brillouin zone (BCD).

00789 (3/3) : 3E @D405 [Chair: Jason Kaye]

## [03564] Density functional theories: reformulations and regularizations

**Format :** Talk at Waseda University

**Author(s) :** Michael Ruggenthaler (Max-Planck Institute for the Structure and Dynamics of Matter)

**Abstract :** Density functional theories try to reformulate quantum theories in terms of a set of reduced quantities, turning high-dimensional linear problems into low-dimensional but non-linear problems (1,2,3). In this talk I will give a short overview of open mathematical problems in density functional theories and provide potential solution strategies, either by Moreau-Yosida regularization (4) or by reformulating the basic mappings (2,3).

- (1) Ruggenthaler, M., Penz, M., & Van Leeuwen, R. (2015). Existence, uniqueness, and construction of the density-potential mapping in time-dependent density-functional theory. *Journal of Physics: Condensed Matter*, 27(20), 203202.
- (2) Penz, M., Tellgren, E. I., Csirik, M. A., Ruggenthaler, M., & Laestadius, A. (2022). The structure of the density-potential mapping. Part I: Standard density-functional theory. *arXiv preprint arXiv:2211.16627*.
- (3) Penz, M., Tellgren, E.I., Csirik, M.A., Ruggenthaler, M, & Laestadius, A (2023). The structure of the density-potential mapping. Part II: Including magnetic fields. *arXiv preprint arXiv:2303.01357*
- (4) Penz, M., Laestadius, A., Tellgren, E. I., & Ruggenthaler, M. (2019). Guaranteed convergence of a regularized Kohn-Sham iteration in finite dimensions. *Physical Review Letters*, 123(3), 037401.

## [04839] Fine-grained parallelism is flow-based Monte Carlo algorithms

**Format :** Talk at Waseda University

**Author(s) :** Michael Samuel Albergo (New York University)Michael S Albergo (New York University)

**Abstract :** Transport-based generative models have become an active topic of inquiry in scientific computing and Monte Carlo-based numerical methods, with demonstrated applications ranging from lattice quantum field theory to molecular systems. In this will talk, I will discuss the flow-based Monte Carlo approach and present some results related to taking advantage of its embarrassingly parallel setup.

## [04906] An unambiguous and robust formulation for Wannier localization

**Format :** Talk at Waseda University

**Author(s) :** Kangbo Li (Cornell University)

**Abstract :** We provide a new variational definition for the spread of an orbital under periodic boundary conditions (PBCs) that is continuous with respect to the gauge, well-suited to diffuse orbitals, and can be adapted for schemes to compute localized Wannier functions. Existing definitions do not satisfy all these desiderata, partly because they depend on an “orbital center”—an ill-defined concept under PBCs. Moreover, we illustrate a more robust and efficient ( $10 \times - 70 \times$  fewer iterations) localization scheme.

# [00792] Recent Advances of Modeling and Computation of Moving Boundary Problems

**Session Time & Room :**

00792 (1/3) : 2C (Aug.22, 13:20-15:00) @D402

00792 (2/3) : 2D (Aug.22, 15:30-17:10) @D402

00792 (3/3) : 2E (Aug.22, 17:40-19:20) @D402

**Type :** Proposal of Minisymposium

**Abstract :** A great number of real-life problems, important for engineering and biological applications, involve time-dependent boundaries, whose motion is controlled by interactions among microscopic and macroscopic driving forces. At the continuum level, one derives models via energy variation approach so that the resulting formulation, usually posed as systems of coupled PDEs and boundary conditions, is consistent with physical laws. To date, grand challenges remain in high-fidelity modeling and efficient computation of these multiscale problems. This minisymposium will (1) address some of most recent topics in modeling and computation; (2) nurture collaborations among investigators in mathematics, biophysics, and engineering.

**Organizer(s) :** Shuwang Li, Yongcheng Zhou, Xiaofan Li

**Classification :** 76D45, 65M22, 92B05, 45B05, 76A10

**Minisymposium Program :**

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00792 (1/3) : 2C @D402

## [01873] Solving motions of an incompressible interface with bending in Navier-Stokes flows

**Format :** Talk at Waseda University

**Author(s) :** Yunchang Seol (Sungkyunkwan University)Ming-Chih Lai (National Yang Ming Chiao Tung University, Taiwan)Kian Chuan Ong (Fields Institute for Research in Mathematical Sciences)Yongsam Kim (Chung-Ang University)

**Abstract :** We present two numerical approaches in the immersed boundary method for solving motions of an incompressible biological cell membrane, a vesicle structure sharing similar behaviors with red blood cells. In the original problem, the surface tension enforcing the interfacial incompressibility is unknown, so the fluid variables and the tension shall be found together via an iterative method which requires huge computational cost. To overcome this difficulty, we introduce a penalty idea and a projection approach.

## [01918] Convergence of boundary integral methods for interfacial Stokes and Darcy flow with surface tension

**Format :** Online Talk on Zoom

**Author(s) :** David M Ambrose (Drexel University)

**Abstract :** We consider efficient numerical methods for interfacial fluid flow. For interfacial Darcy flow in three space dimensions and interfacial Stokes flow in two space dimensions, we demonstrate convergence of boundary integral methods. The problems are subject to the effect of surface tension and/or elastic membrane forces. The proofs rely on energy estimates. This will include joint work with Yang Liu, Michael Siegel, Svetlana Tlupova, and Keyang Zhang.

## [02287] A Cartesian Grid-Based Boundary Integral Method for Moving Interface Problems

**Format :** Talk at Waseda University

**Author(s) :** Han Zhou (Shanghai Jiao Tong University)Wenjun Ying (Shanghai Jiao Tong University)

**Abstract :** Moving interface problems are ubiquitous in natural sciences. Often the interface motion is coupled with PDEs in the bulk domain. This talk will present a Cartesian grid-based boundary integral method for solving

moving interface problems. Layer potentials are evaluated by solving simple interface problems on a Cartesian grid to take advantage of fast solvers such as FFTs and the geometric multigrid method. Numerical simulations, including crystal growth and two-phase flows, will be reported.

## [02762] An explicit numerical method for the Cahn-Hilliard equation

**Format :** Talk at Waseda University

**Author(s) :** Junseok Kim (Korea University) Soobin Kwak (Korea University)

**Abstract :** In this talk, I present an explicit conservative numerical method for the Cahn–Hilliard (CH) equation, which is a famous mathematical model for conservative phases. The CH equation has been applied in many important problems and a lot of computational methods were developed to numerically compute the CH equation. So far most of numerical methods were based on implicit numerical methods because of very stiff timestep restriction of the explicit scheme. To overcome this severe time-step restriction of the explicit scheme, we developed an explicit conservative numerical scheme. To demonstrate the superior performance of the proposed scheme, we present the computational experiments.

00792 (2/3) : 2D @D402

## [02792] Viscous fingers in a Hele-Shaw cell under an electric field

**Format :** Talk at Waseda University

**Author(s) :** Meng Zhao (Huazhong University of Science and Technology)

**Abstract :** We investigate the nonlinear dynamics of a moving interface in a Hele-Shaw cell subject to an in-plane applied electric field. We develop a spectrally accurate numerical method for solving a coupled integral equation system. Our nonlinear results reveal that currents are able to promote/suppress the interface dynamics depending on its direction. When no fluid is injected, and a negative current is utilized, the interface tends to approach the origin and break up into several drops.

## [02813] Computing viscoelastic and elastoplastic deformations induced by volumetric growth

**Format :** Talk at Waseda University

**Author(s) :** Min Wu (Worcester Polytechnic Institute)

**Abstract :** Based on a discretized energy formulation, I will present a numerical method to solve various nonlinear mechanical systems involving finite elastic deformation, Maxwell-type viscoelasticity, or elastoplasticity. I will show its application to simulate deformations of living and nonliving soft materials during volumetric growth with free boundaries. These simulations can give insight into swelling gel experiments, in vitro wound closure dynamics, and cell and tissue morphogenesis.

## [02818] Disturbance flow generated by particles in linear viscoelastic fluids

**Format :** Talk at Waseda University

**Author(s) :** Xiaofan Li (Illinois Institute of Technology) Hualong Feng (California State Univ, Bakersfield) Amlan Barua (Indian Institute of Technology Dharwad) Shuwang Li (Illinois Institute of Technology)

**Abstract :** Studying effects of moving particles on fluids is of fundamental importance for understanding particle dynamics and binding kinetics. We compute the fluid dynamics using an accurate boundary integral method with 3rd order accuracy in space. A unique feature of our method is that we can calculate the stress on the particle surface for a prescribed particle velocity profile. It is well known that a boundary layer develops along an infinite plate under oscillatory motion in a Newtonian fluid. When the flow becomes viscoelastic, however, the boundary layers are fundamentally different than those observed in Newtonian fluids.

## [02820] Mathematical Modeling and Computation of Tumor Growth

**Format :** Online Talk on Zoom

**Author(s) :** Min-Jhe Lu (University of California, Irvine) John Lowengrub (University of California, Irvine) Chun Liu (Illinois Tech) Shuwang Li (Illinois Tech) Yiwei Wang (University of California, Riverside)

**Abstract :** The building of the mechano-chemical tumor models aims to understand how the mechanical interaction and the biochemical reactions can influence the dynamics of tumor growth. The mechanical interaction within cells produces stress and the biochemical reactions involve chemical species supplying tumor with nutrients. In this talk I will demonstrate how we build the tumor models with energetic variational

part\_2

approaches and the numerical simulation results in both sharp interface and diffuse interface formulation will also be given.

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00792 (3/3) : 2E @D402

### [02821] Hydrodynamics of Tunable Janus Particles

**Format :** Online Talk on Zoom

**Author(s) :** Rolf Josef Ryham (Fordham University)Yuan Nan Young (New Jersey Institute of Technology)Bryan Quaife (Florida State University)Szu-Pei Fu (Trinity College)

**Abstract :** We use a model recently developed for the many-body hydrodynamics of amphiphilic JPs under a viscous background flow to investigate distinct particle phases that arise when accounting for asymmetric and polar hydrophobes. We quantify the macroscopic properties of novel JP phases under a linear shear and a Taylor-Green mixing background flow and quantify their macroscopic, complex-fluid behavior. These numerical results provide insight into dynamic control of non-equilibrium active biological systems with similar self-organization.

### [02823] Sharp interface problem of Ohta-Kawasaki Model

**Format :** Talk at Waseda University

**Author(s) :** Amlan K Barua (IIT Dharwad)

**Abstract :** The Ohta Kawasaki (OK) model investigates mesoscopic phase separation in block copolymers. In this talk, we discuss a sharp interface version of OK equations using matched asymptotic expansions. The resultant equations resemble a Hele-Shaw type system. We suggest a boundary integral formulation of the problem and propose highly accurate numerical techniques to solve the equations. We conduct long-time simulation using our numerical methods. The simulation results show the emergence of various interesting configurations.

### [02835] Phase-field modeling and simulation of controllable dendritic growth

**Format :** Talk at Waseda University

**Author(s) :** Darae Jeong (Kangwon National University)

**Abstract :** In this study, we consider the controllable dendritic growth model with phase-field method. The governing system consists of three equations that are for capturing the interface between solid and melt phases, diffusion of the temperature, and structure by molecular orientations in solid. We propose the time-dependent adaptive mesh and finite-difference algorithm, which is designed to efficiently solve the governing system. After that, we present several numerical simulation to show the various patterns and its corresponding parameter effect for crystal formation. And we demonstrate the effectiveness of our approach by comparing numerical results with other method.

## [00793] SIAM Student Chapter Research Presentations

**Session Time & Room :**

00793 (1/3) : 2E (Aug.22, 17:40-19:20) @E818

00793 (2/3) : 3C (Aug.23, 13:20-15:00) @E818

00793 (3/3) : 3D (Aug.23, 15:30-17:10) @E818

**Type :** Proposal of Minisymposium

**Abstract :** The SIAM Student Chapter Research Presentations minisymposium is designed to encourage student participation, to meet with both peers and professionals in their field and to promote interaction between newly established Student Chapters in the East Asia Section. The presentations given by students include recent advances in applied mathematics and computational science. Organizers also hope to encourage those in the learning community to establish new student chapters of SIAM and to strengthen collaboration opportunities between students and the SIAM leadership.

**Organizer(s)** : Tulin Kaman, Eric Chung

**Classification** : 68Txx, 70Kxx, 62Dxx, Machine Learning, Nonlinear Dynamics, Statistical Sampling Theory

**Minisymposium Program :**

00793 (1/3) : 2E @E818

## [03324] Continuum Limit of Nonlocal Diffusion on Inhomogeneous Networks

**Author(s)** : Itsuki Watanabe (Waseda University)

**Abstract** : We present two limit theorems for the zero-range process with nonlocal diffusion on inhomogeneous networks. The deterministic model is governed by the reaction-diffusion equation with an integral term in space instead of a Laplacian. By constructing the reproducing kernel Hilbert space to consider the inhomogeneities of the network structure, we prove that the law of large numbers and the central limit theorem hold for our models.

## [03390] Computing the invariant measure of the N-vortex problem on the sphere by Hamiltonian Monte Carlo

**Author(s)** : Kota Takeda (Kyoto University)Takashi Sakajo (Kyoto University)

**Abstract** : We consider Hamiltonian Monte Carlo(HMC) to approximates a given target distribution on manifolds embedded in Euclidean space. Its efficiency is guaranteed by the exponential convergence property called geometric ergodicity. We have proven that HMC has geometric ergodicity for smooth distributions on compact manifolds. As an application, we compute the invariant measure of the N-vortex problem on the unit sphere by HMC.

## [03516] REGULARIZED ADAPTIVE HUBER MATRIX REGRESSION AND DISTRIBUTED LEARNING

**Author(s)** : YUE WANG (City University of Hong Kong)

**Abstract** : Matrix regression provides a powerful technique for analyzing matrix-type data, as exemplified by many contemporary applications. Despite the rapid advance, distributed learning for robust matrix regression to deal with heavy-tailed noises in the big data regime still remains untouched. In this paper, we first consider adaptive Huber matrix regression with a nuclear norm penalty, which enjoys insensitivity to heavy-tailed noises without losing statistical accuracy. To further enhance the scalability in massive data applications, we employ the communication-efficient surrogate likelihood framework to develop distributed robust matrix regression, which can be efficiently implemented through the ADMM algorithms. Under only bounded  $(1 + \delta)$ -th moment on the noise for some  $\delta \in (0, 1]$ , we provide upper bounds for the estimation error of the central estimator and the distributed estimator and prove they can achieve the same rate as established with sub-Gaussian tails when only the second moment of noise exists. Numerical studies verify the advantage of the proposed method over existing methods in heavy-tailed noise settings.

## [03650] Optimal Contextual Bandits with Knapsacks under Realizability via Regression Oracles

**Author(s)** : Jialin ZENG (Hong Kong University of Science and Technology)Yuxuan HAN (Hong Kong University of Science and Technology)Yang WANG (Hong Kong University of Science and Technology)Yang XIANG (Hong Kong University of Science and Technology)Jiheng ZHANG (Hong Kong University of Science and Technology)

**Abstract** : We study the stochastic contextual bandit with knapsacks (CBwK) problem, where each action, taken upon a context, not only leads to a random reward but also costs a random resource consumption in a vector form. The challenge is to maximize the total reward without violating the budget for each resource. We study this problem under a general realizability setting where the expected reward and expected cost are functions of contexts and actions in some given general function classes F and G, respectively. Existing works on CBwK are restricted to the linear function class since they use UCB-type algorithms, which heavily rely on the linear form and thus are difficult to extend to general function classes. Motivated by online regression oracles that have been successfully applied to contextual bandits, we propose the first universal and optimal algorithmic framework for CBwK by reducing it to online regression. We also establish the lower regret bound to show the optimality of our algorithm for a variety of function classes.

## [03692] Differentially Private Confidence Interval for Extrema of Parameters

**Author(s)** : Xiaowen Fu (Hong Kong University of Science and Technology)Yang Xiang (Hong Kong University of Science and Technology)Xinzhou Guo (Hong Kong University of Science and Technology)

**Abstract** : We aim to construct a valid and efficient confidence interval for the extrema of parameters under privacy protection. The usual statistical inference on the extrema of parameters often suffers from the selection bias issue, and the problem becomes more acute, as in many application scenarios of extrema parameters, we often need to protect the privacy of the data. In this work, we focus on the exponential family of distributions and propose a privatized parametric bootstrap method to address selection bias in the extrema of parameters problem under the scheme of differential privacy. While the usual privatized parametric bootstrap does not address selection bias appropriately, we prove that with a privatized bias correction term, the proposed parametric bootstrap method can lead to a valid and efficient confidence interval for the extrema of parameters. We illustrate the proposed method with the Gaussian case and regression case and demonstrate the advantages of the proposed method via numerical experiments and real data examples.

## [03749] Spherical signal processing via framelets and convolutional neural networks

**Author(s)** : Jianfei Li (City University of Hong Kong)

**Abstract** : In this talk, we would like to introduce a general theoretical framework for constructing Haar-type tight framelets on any compact set with a hierarchical partition. In particular, we develop novel spherical framelets with directionality and combine them with CNNs for image denoising and inpainting tasks. The experiment results show that our proposed CNN model outperforms threshold methods.

## [03813] O(N) dense direct factorization with near-perfect weak scaling.

**Author(s)** : Sameer Satish Deshmukh (Tokyo Institute of Technology)Rio Yokota (Tokyo Institute of Technology)George Bosilca (University of Tennessee at Knoxville)

**Abstract** : Approximating the off-diagonal blocks of dense matrices arising from the Boundary Element Method can reduce the time of a dense direct factorization from  $O(N^3)$  to  $O(N)$  with controllable error.

Distributed factorization of such algorithms is challenging due to the presence of small, irregular computations. In this talk, we show how asynchronous execution can achieve good weak scaling on FUGAKU for a variety of Green's functions on a 2D geometry.

## [03907] Distributed Optimization with Imperfect Communication

**Author(s)** : Jie Liu (City University of Hong Kong)

**Abstract** : In distributed optimization over multi-agent networks, each agent is endowed with a local private objective function. The purpose of distributed optimization is to minimize the sum of all agents' local objective functions cooperatively through information communication between different agents. However, the communication channels in the real life are not always perfect due to limited data rates, communication delays, noises, etc. In this presentation, we shall discuss distributed optimization with imperfect communication.

## [04039] SPHERICAL FRAMELETS FROM SPHERICAL DESIGNS

**Author(s)** : Yuchen XIAO (City University of Hong Kong)

**Abstract** : In this paper, we investigate in detail the structures of the variational characterization  $A_{N,t}$  of the spherical  $t$ -design, its gradient  $\nabla A_{N,t}$ , and its Hessian  $H(A_{N,t})$  in terms of fast spherical harmonic transforms. Moreover, we propose solving the minimization problem of  $A_{N,t}$  using the trust-region method to provide spherical  $t$ -designs with large values of  $t$ . Based on the obtained spherical  $t$ -designs, we develop (semi-discrete) spherical tight framelets as well as their truncated systems and their fast spherical framelet transforms for the practical spherical signal/image processing. Thanks to the large spherical  $t$ -designs and localization property of our spherical framelets, we are able to provide signal/image denoising using local thresholding techniques based on a fine-tuned spherical cap restriction. Many numerical experiments are conducted to demonstrate the efficiency and

effectiveness of our spherical framelets, including Wendland function approximation, ETOPO data processing, and spherical image denoising.

## [04179] Introducing Deep Unfolding: Incorporating Prior Knowledge into Deep Learning Models

**Author(s)** : Yumeng REN (City University of Hong Kong)

**Abstract** : Deep unfolding (DU) methods accelerate iterations for inverse problems by incorporating prior knowledge into deep learning models, which can be based on backbone iterations such as the ADMM algorithm for reconstruction tasks and a PDE discretization scheme for learning PDEs from data. In this talk, I will introduce the basics of DU methods, ADMM-type backbone iterations and recent advances.

## [05002] Koopman analysis and Dynamic mode decomposition of Elementary Cellular Automata

**Author(s)** : Keisuke Taga (Waseda University)Yuzuru Kato (Future University Hakodate)Yoshihiro Yamazaki (Waseda University)Hiroya Nakao (Tokyo Institute of Technology)

**Abstract** : We perform Koopman spectral analysis and Dynamic mode decomposition (DMD) for Elementary Cellular Automata (ECA). Koopman operator is a linear operator describing the time evolution of observables of a dynamical system, and DMD is a data-driven approach to Koopman analysis. ECA is the simplest example of finite-state systems that describe spatiotemporal patterns and, thus, a good testbed for assessing the performance of DMD. We report the reproducibility of the dynamics and spectral properties of ECA by different DMD algorithms and explain the linear algebraic background.

# [00794] Mathematical Modelling and Disease

**Session Time & Room** : 2E (Aug.22, 17:40-19:20) @A512

**Type** : Proposal of Minisymposium

**Abstract** : Mathematical modeling and estimation strategies are especially useful in the fight against disease be it through diagnosis, prediction, or management. Examples include analyzing medical device performance and providing simulation, constructing probabilistic/stochastic models that define classification strategies that in turn guide diagnostic testing. In this minisymposium, these themes will be investigated through specific ‘real world’ examples emphasizing metrology and the importance of measurement science in using mathematics to treat disease.

**Organizer(s)** : Anthony Kearsley, Luis Melara

**Classification** : 92-10, 92-08, 92C75

**Minisymposium Program** :

00794 (1/1) : 2E @A512 [Chair: Luis Melara]

## [01627] Transboundary management of ecological systems with applications to diseases

**Format** : Talk at Waseda University

**Author(s)** : Julie Blackwood (Williams College)

**Abstract** : Human migration and infectious diseases often span multiple administrative jurisdictions that might have different systems of government and management objectives. I'll introduce two examples in which spatial coordination may be critical for disease control. First, I'll demonstrate that spatial interactions of vampire bats likely play a key role in driving rabies persistence. Second, I'll describe a more general infectious disease in humans and show that successful management may depend on the actions of multiple managers.

## [04446] Separating Populations in Flow Cytometry Experiments: A Probabilistic Approach

**Format :** Talk at Waseda University

**Author(s) :** Danielle J Middlebrooks (National Institute of Standards and Technology)

**Abstract :** Flow cytometry (FC) is used in many areas of clinical testing, measuring cell characteristics of roughly one million cells. Data analysis is critical for interpreting FC measurements, but traditional techniques are often time-consuming and subjective. Our methodology identifies an unknown population by constructing probability density functions of specific biomarker expression levels in a sample. Once we estimate the unknown distribution, we compute the relative fraction of the unknown population and estimates of the uncertainty.

## [04840] Case Studies in Modeling and Optimization for Diagnostics

**Format :** Talk at Waseda University

**Author(s) :** Prajakta Purushottam Bedekar (National Institute of Standards and Technology)Paul Patrone (National Institute of Standards and Technology)Anthony Kearsley (National Institute of Standards and Technology)

**Abstract :** We demonstrate that modeling and optimization are crucial tools for interpretation of diagnostic measurements through case studies. First we model the errors in dilution and find a best-fit to minimize variability of biological antibody measurements, enabling us to compare results across experiments. Secondly, we use optimal decision theory to develop a time-dependent, probabilistic classification and adaptive prevalence estimation scheme using antibody testing measurements. We demonstrate the results by using SARS-CoV-2 datasets.

## [03298] Optimal Bandwidth Selection in Bio-FET Measurements

**Format :** Talk at Waseda University

**Author(s) :** Luis Melara (Shippensburg University)

**Abstract :** The use of stochastic regression to separate signal from noise produced by Bio-FETs will be discussed in this talk. The noise realized by BioFETs interferes with quantitative and qualitative analysis, thus determining optimal bandwidth associated with experimental Bio-FET data measurements is an important task. Presented results suggest consistent across aspect ratios and a choice of stochastic regression kernel function and yield what appear to be good results.

## [00795] Topological data analysis and machine learning

**Session Time & Room :**

00795 (1/3) : 1C (Aug.21, 13:20-15:00) @G301

00795 (2/3) : 1D (Aug.21, 15:30-17:10) @G301

00795 (3/3) : 1E (Aug.21, 17:40-19:20) @G301

**Type :** Proposal of Minisymposium

**Abstract :** Topological Data Analysis (TDA), a relatively new field of data analysis, has proved highly useful in a variety of applications. Recently, much TDA research has been devoted to not only developing theories but also developing TDA compatible in machine learning workflow. This workshop will bring together researchers working on the areas of TDA and machine learning and provide an opportunity where they present their recent research and share ideas both in theory and applications. Further, this workshop will also provide recent progresses of computational tools developed for TDA combined with machine learning in various applications.

**Organizer(s) :** Jae-Hun Jung, Shizuo Kaji, Moo K. Chung

**Classification :** 00A65, 55N31

**Minisymposium Program :**

00795 (1/3) : 1C @G301 [Chair: Moo K. Chung]

## [03334] Topological Data Analysis of Spatial Systems

**Format :** Talk at Waseda University

**Author(s) :** Mason Alexander Porter (UCLA)

**Abstract :** I discuss several applications of topological data analysis to spatial systems. I will consider examples from voting, city streets, the spread of COVID-19.

## [03341] Bigraded persistence barcodes and their stability

**Format :** Talk at Waseda University

**Author(s) :** Anthony Bahri (Rider University)Ivan Limonchenko (Higher School of Economics)Taras Evgenievich Panov (Moscow State University)Jongbaek Song (Pusan National University)Donald Stanley (University of Regina)

**Abstract :** We define the bigraded persistent homology modules and the bigraded barcodes of a finite pseudo-metric space  $X$  using the ordinary and double homology of the moment-angle complex associated with the Vietoris-Rips filtration of  $X$ . Then we discuss the stability for the bigraded persistent double homology modules and corresponding bigraded barcodes.

## [03617] Learning visual representation with homological labels

**Format :** Talk at Waseda University

**Author(s) :** Shizuo Kaji (Kyushu University)Yohsuke Watanabe (ZOZO inc.)

**Abstract :** We propose a new scheme for convolutional neural networks to learn visual representation with synthetic images and mathematically-defined labels that capture topological information. Our scheme can be viewed as a type of self-supervised learning, where the regression of vectorised persistent homology of an image is learned. We show that the acquired visual representation supplements the one obtained by the usual supervised learning with manually-defined labels by confirming an improved convergence in training for image classification. Our method provides a simple way to encourage the model to learn global features through a specifically designed task based on topology. It requires no real images nor manual labels and can be utilised at a minimal extra cost.

## [03647] Exact multi-parameter persistent homology of time-series data: Fast and variable one-dimensional reduction of multi-parameter persistence theory

**Format :** Talk at Waseda University

**Author(s) :** Keunsu Kim (POSTECH)Jae-Hun Jung (POSTECH)

**Abstract :** Time-series data can be inferred as a periodic signal, enabling a continuous approximation with discrete Fourier transform to reveal the relation between its Fourier modes and topology of the data. We introduce an exact multi-parameter persistent homology construction utilizing the fast Fourier transform and Künneth formula, which computes and interprets the corresponding persistent barcode in a fast and efficient manner. This work is based on <https://arxiv.org/abs/2211.03337>

00795 (2/3) : 1D @G301 [Chair: Shizuo Kaji]

## [03657] Generic transitions for flows on surfaces with or without constraints

**Format :** Talk at Waseda University

**Author(s) :** Tomoo Yokoyama (Saitama University)

**Abstract :** This talk describes the generic time evolutions of gradient flows and Hamiltonian flows on surfaces with or without physical constraints. Moreover, we show the non-contractibility of connected components of the spaces of such flows, respectively, under the non-existence of creations and annihilations of singular points by using combinatorics and simple homotopy theory.

## [04624] Topological learning for multiscale biology

**Format :** Talk at Waseda University

**Author(s) :** Heather Harrington (University of Oxford)

**Abstract :** Biological processes are multi-scale. Spatial structures and patterns vary across levels of organisation, from molecular to multi-cellular to multi-organism. With more sophisticated mechanistic models and data available, quantitative tools are needed to study their evolution in space and time. The most prominent tool in

topological data analysis is persistent homology (PH), which provides a multi-scale summary of data. Here we present extensions to the PH pipeline and highlight its utility with concrete case studies.

## [04715] Topological Data Analysis for Biological Images and Video

**Format :** Online Talk on Zoom

**Author(s) :** Peter Bubenik (University of Florida)

**Abstract :** I will present the results of two projects applying topological data analysis (TDA) and machine learning (ML) to biological data. In the first, we have developed a tool, TDAExplore, that combines TDA and ML to both classify biological images and to provide a visualization that is biologically informative. In the second, we use TDA and ML to classify quasi-periodic biological videos and we apply TDA to such a video to produce synthetic periodic videos.

## [05453] Topological data analysis of music data and AI composition

**Format :** Talk at Waseda University

**Author(s) :** Jae-Hun Jung (POSTECH)Mai Lan Tran (POSTECH)Dongjin Lee (POSTECH)

**Abstract :** We employ topological data analysis to analyze music. Initially, the provided music data is transformed into a graph and we identify embedded cycles within the music using persistent homology. We elucidate how the cycle structure changes based on the metric definition between music nodes, with theoretical justifications. Then, we introduce the overlap matrix, which shows the interconnectedness of these cycles. We explain an AI algorithm utilizing the overlap matrix to facilitate new music compositions.

00795 (3/3) : 1E @G301 [Chair: Jae-Hun Jung]

## [05456] GRIL: A 2-parameter Persistence Based Vectorization for Machine Learning

**Format :** Talk at Waseda University

**Author(s) :** Soham Mukherjee (PhD Student)Tamal Krishna Dey (Purdue University)

**Abstract :** 1-parameter persistent homology, a cornerstone in Topological Data Analysis (TDA), studies the evolution of topological features such as connected components and cycles hidden in data. It has been applied to enhance the representation power of deep learning models, such as Graph Neural Networks (GNNs). To enrich the representations of topological features, here we propose to study 2-parameter persistence modules induced by bi-filtration functions. In order to incorporate these representations into machine learning models, we introduce a novel vector representation called Generalized Rank Invariant Landscape (GRIL) for 2-parameter persistence modules. We show that this vector representation is 1-Lipschitz stable and differentiable with respect to underlying filtration functions and can be easily integrated into machine learning models to augment encoding topological features. We present an algorithm to compute the vector representation efficiently. We also test our methods on synthetic and benchmark graph datasets, and compare the results with previous vector representations of 1-parameter and 2-parameter persistence modules.

## [05457] Topological Classification of Zero Sum Games

**Format :** Talk at Waseda University

**Author(s) :** Alexander Strang (University of Chicago)

**Abstract :** Zero-sum two-player games are widely used to model competitive interactions in biology, economics, and reinforcement learning. Unlike classical game theory, which focuses on optima, empirical game theory studies the structure of games and decision problems via observations of play by a population. We study a classification scheme for games based on their topology after embedding into a latent space. Using observed interactions, we infer the spectrum of the payout function when treated as the kernel of an integral operator. The eigenfunctions of the operator can be used to embed agents. The embedded agents form a scatter cloud whose topology provides a natural framework for classifying games. We study the classification of a series of randomly generated extensive form games and decision problems.

## [05458] Topological Embedding of Brain Networks for Differentiating Temporal Lobe Epilepsy

**Format :** Talk at Waseda University

**Author(s) :** Moo K Chung (University of Wisconsin-Madison)

**Abstract :** In this study, we approach the discrimination of functional brain networks in temporal lobe epilepsy patients from those of healthy controls through persistent homology. Starting with a weighted graph, we perform a graph filtration, yielding the birth-death decomposition. This process allows us to uniquely decompose each graph into two subgraphs characterized by 0D and 1D topology. The 0D subgraph arises from the birth of connected components, whereas the 1D subgraph manifests through the death of 1-cycles during the filtration. The distinguishing features of each graph are thus represented by the sorted birth and death values. To compare multiple weighted graphs, we propose a topological version of multidimensional scaling, which embeds these graphs into a 2D plane. This technique offers potential insights for resting-state functional magnetic resonance imaging (rs-fMRI) studies, particularly in distinguishing the functional brain networks associated with temporal lobe epilepsy. This presentation draws upon the findings from the paper available on arXiv:2302.06673.

## [05459] Barcodes and Kernels for multiparameter persistence

**Format :** Online Talk on Zoom

**Author(s) :** Mathieu Carrière (Centre Inria d'Université Côte d'Azur)

**Abstract :** Multiparameter persistence is a generalization of persistent homology that allows for more than a single filtration function. Such constructions arise naturally when considering data with outliers or variations in density, time-varying data, or functional data.

In single-parameter persistence, the barcode is equivalent to the “rank invariant”: the function that associates the rank of the corresponding linear map to every pair of comparable points. However, nearly all of the tools developed in persistent homology are based on the barcode. This is because it is a concise and geometric descriptor that lends well to data analysis and visualization. Therefore, it is crucial, and perhaps imperative, to construct a generalized barcode to work with the rank-invariant for multiparameter persistence efficiently.

Perhaps surprisingly, recent work has shown that if we allow the elements of the barcode to be signed intervals, then such a generalization is possible. I will discuss how one can use homological algebra to obtain a signed barcode in a stable manner. Furthermore, I will discuss how signed barcodes can be used in machine learning pipelines and report on recent computational results obtained using generalizations of the so-called sliced Wasserstein kernel to such signed barcodes.

## [00802] Numerical Algorithms for the Eikonal Equation and Its Applications

**Session Time & Room :**

00802 (1/3) : 2D (Aug.22, 15:30-17:10) @F402

00802 (2/3) : 2E (Aug.22, 17:40-19:20) @F402

00802 (3/3) : 3C (Aug.23, 13:20-15:00) @F402

**Type :** Proposal of Minisymposium

**Abstract :** The minisymposium focuses on the recent state-of-art for the eikonal equation in view of the mathematical theories, diverse applications such as image processing, seismic wave travel time in layered media, 3D shape reconstruction, 3D printing, optimal control, homogenization, mean field games, and distance on a non-convex domain with polyhedral meshes, and their numerical algorithms; semi-discretization method, finite volume method, mimetic discretization method, using the Hopf-Lax formula, Jet marching method, variational methods, neural network approaches, etc. We also include a variant of the eikonal partial differential equation induced by Randers metric and a high order accurate efficient eikonal solvers on surfaces.

**Organizer(s) :** Jooyoung Hahn, Laurent Cohen

**Classification :** 49L25, 35D40, 65N22

**Minisymposium Program :**

## [03439] Eikonal methods applied to image segmentation

**Format :** Talk at Waseda University

**Author(s) :** Laurent D. Cohen (CEREMADE, Universite Paris dauphine, PSL, CNRS)

**Abstract :** Minimal paths have been used for long as an interactive tool to find contours or segment tubular and tree structures, like vessels in medical images. These minimal paths correspond to minimal geodesics according to some relevant metric defined on the image domain. Finding a geodesic distance and geodesic paths can be solved by the Eikonal equation using the fast and efficient Fast Marching method. We will present various applications to image segmentation.

## [04713] Casualty and anisotropy in the design of eikonal solvers

**Format :** Talk at Waseda University

**Author(s) :** Jean-Marie Mirebeau (Centre Borelli, CNRS, ENS Paris-Saclay)

**Abstract :** The eikonal equation characterizes the arrival time of a front, propagating at a speed which is locally dictated by the front position and normal direction, and which crucially is always positive.

The causality property is the discrete counterpart of the monotonic progression of the front, and is at the foundation of efficient numerical solvers of the eikonal equation such as the fast marching method. I will describe an eikonal solver enjoying this property and applying to the tilted transversely anisotropy encountered in some geological media, as well as recent efforts on the formalization of the causality property, and its application to models which advect a state.

## [03987] Learning to Measure Distances: High Order Accurate Efficient Eikonal Solvers on Surfaces

**Format :** Talk at Waseda University

**Author(s) :** Ron Kimmel (Technion - Israel Institute of Technologyn )

**Abstract :** The intimate relation between Eikonal equations and distance maps would be our starting point. When introducing a numerical solver, the balance between accuracy and complexity is at the core of computer science and a measure of quality of our solution. We will present a high accuracy deep learning method for approximating geodesic distances on surfaces at linear computational complexity. For training an accurate local solver a bootstrapping mechanism is employed.

## [03578] An Artificial Neural Network Approach for Re-distancing Implicit Surfaces

**Format :** Talk at Waseda University

**Author(s) :** Yesom Park (Seoul National University)Chang hoon Song (Seoul National University)Jooyoung Hahn (Slovak University of Technology in Bratislava)Myungjoo Kang (Seoul National University)

**Abstract :** Following the success of machine learning tasks, the use of neural networks for solving PDEs has begun to show promising results. In this talk, we introduce a deep-learning-based method for recovering the signed distance function (SDF) from an implicit level set function representation of the hypersurface. By exploiting one of the main advantages of neural network approaches which is flexibility in network design and optimization objectives, our developments have two-fold: First, in order to increase the expressiveness of the network, we propose an augmented network that parameterizes the SDF together with the gradient of SDF as an auxiliary output while keeping the number of parameters. Second, we introduce a new objective that exploits a more global property and regularizes the singularity of the SDF by harnessing the geometric properties of the SDF. Numerical experiments on a diverse range of interfaces on two and three-dimensional domains validate the effectiveness and accuracy of the proposed method.

00802 (2/3) : 2E @F402 [Chair: Jooyoung Hahn]

## [03777] Approximate viscosity solutions of hamilton-Jacobi equations: a review

**Format :** Online Talk on Zoom

**Author(s) :** Italo Capuzzo Dolcetta Italo (Sapienza Università di Roma)

**Abstract :** Semi-discretization methods to approximate viscosity solutions of Hamilton-Jacobi equations arising in different applied contexts such as optimal control, shape from shading, homogenization, and mean field games

## [04731] Eikonal equation in 3D shape reconstruction and 3D printing

**Format :** Online Talk on Zoom

**Author(s) :** Silvia Tozza (Dept. of Mathematics, University of Bologna)

**Abstract :** The topic of this talk is related to Hamilton-Jacobi equations and their numerical resolution in the context of Image Processing. More in details, we will deal with the 3D reconstruction of the shape of an object (the resolution of the so-called Shape-from-Shading problem via a differential approach) and some problems related to 3D printing of the reconstructed object. In particular cases, the Hamilton-Jacobi equation describing these problems reduces to the eikonal equation.

## [04972] The redistancing problem using Hopf-Lax formula and its applications

**Format :** Talk at Waseda University

**Author(s) :** Byungjoon Lee (The Catholic University of Korea)

**Abstract :** The redistancing, or reinitialization, problem is an important subject when one considers the signed distance function to the interface. There have been many researches on redistancing a given function to a signed distance function, based on numerical methods to solve the following eikonal equation:

$$\frac{\partial \phi}{\partial t}(x, t) + \|\nabla_x \phi(x, t)\|_2 = 0, \quad (x, t) \in \mathbb{R}^n \times (0, \infty)$$

In this talk, we review the novel redistancing technique based on Hopf-Lax formula equipped with the split Bregman approach and discuss on its applications.

## [04630] Comparison study of image-segmentation techniques by a curvature-driven flow of planes curves

**Format :** Talk at Waseda University

**Author(s) :** Shigetoshi Yazaki (Meiji University)

**Abstract :** In this talk, we deal with image segmentation by a curvature-driven flow of curves in the plane.

We focus on images in the plane. Several methods to image segmentation are discussed.

For instance, the minimum radius method, L2-gradient flow method, stepwise method, etc.

Then, all methods are compared in the qualitative computational study.

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00802 (3/3) : 3C @F402 [Chair: Laurent D. Cohen]

## [03535] Variational methods for distance function approximation and applications

**Format :** Talk at Waseda University

**Author(s) :** Pierre-Alain Fayolle (University of Aizu)Alexander Belyaev (Heriot-Watt University)

**Abstract :** The distance function (signed or unsigned) to the boundary (curve or surface) of a given geometric domain is a useful tool in geometry processing, shape and solid modeling, as well as other related domains. It has various applications in several fields including surface reconstruction from scattered data, meshing, shape interrogation, computational fluid dynamics (turbulence modeling), computational mechanics, and robot path planning. In this talk, I will focus on several recent variational methods for computing the distance function or its approximation. Efficient numerical algorithms corresponding to these methods will also be discussed.

## [02323] Solving the eikonal equation utilizing mimetic methods

**Format :** Talk at Waseda University

**Author(s) :** Miguel Dumett (San Diego State University)

**Abstract :** The Eikonal equation with Soner boundary conditions is solved utilizing high-order mimetic differences. Mimetic difference methods construct PDE discrete analogs. These preserve vector calculus identities as well as its integral theorems while keeping constant order of accuracy over the whole grid, including the boundary. The proposed algorithm leverages on the Fast Marching method and resembles a quasi-Newton iterative scheme.

## [03845] Jet marching on unstructured meshes: algorithms and applications

**Format :** Talk at Waseda University

**Author(s) :** Samuel F Potter (Courant Institute of Mathematical Sciences)

**Abstract :** The jet marching method (JMM) solves the eikonal equation by marching its jet using semi-Lagrangian updates (i.e., local raytracing). Marching jets enables a compact Hermite interpolation-based scheme, enabling the use of paraxial raytracing for marching the amplitude of the associated geometric optic wave. We use the JMM to solve high-frequency wave problems on unstructured meshes, with applications motivated by computational room acoustics and light transport in miniwasp ommatidia.

## [03445] Regularized eikonal equation on polyhedral meshes

**Format :** Talk at Waseda University

**Author(s) :** Jooyoung Hahn (Slovak University of Technology in Bratislava) Karol Mikula (Slovak University of Technology in Bratislava) Peter Frolkovič (Slovak University of Technology in Bratislava)

**Abstract :** A cell-centered finite volume method (FVM) is discussed to compute a distance from objects on a 3D computational domain discretized by polyhedral cells. Time-relaxed and Laplacian-regularized eikonal equations are compared numerically and we show how the Soner boundary condition is straightforwardly combined in a conventional FVM code. The Laplacian regularization is more practical for large numbers of cells or distant regions of interest. Additionally, the algorithms can be implemented with parallel computing using domain decomposition.

# [00810] Recent Developments on the Numerical Solution of Least Squares Problems

**Session Time & Room :**

00810 (1/3) : 1C (Aug.21, 13:20-15:00) @E508

00810 (2/3) : 1D (Aug.21, 15:30-17:10) @E508

00810 (3/3) : 1E (Aug.21, 17:40-19:20) @E508

**Type :** Proposal of Minisymposium

**Abstract :** Talks will be presented on recent developments in the numerical solution of least squares problems. Topics included are, numerical solution of least squares problems including preconditioners, rank-deficient and singular systems, quaternion least squares problems, total least squares problems including condition numbers and quantum-inspired algorithms, randomized algorithms such as the randomized Kaczmarz method, and regularization methods for the solution of ill-posed problems.

**Organizer(s) :** Ken Hayami, Yimin Wei

**Classification :** 65F10, 65F20, 65F08, 65F22, 68W20

**Minisymposium Program :**

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00810 (1/3) : 1C @E508 [Chair: Ken Hayami]

## [01652] MinAres: An Iterative Solver for Symmetric Linear Systems

**Format :** Talk at Waseda University

**Author(s) :** Alexis Montoison (GERAD and Polytechnique Montréal) Dominique Orban (GERAD and Polytechnique Montréal) Michael Saunders (Stanford University)

**Abstract :** We introduce an iterative solver named MinAres for symmetric linear systems  $Ax \approx b$ , where  $A$  is possibly singular.

MinAres is based on the symmetric Lanczos process, like Minres and Minres-QLP, but it minimizes  $\|Ar_k\|$  in each Krylov subspace rather than  $\|r_k\|$ , where  $r_k$  is the current residual vector.

In our experiments, MinAres terminates significantly earlier than Minres on ill-conditioned and singular linear systems.

## [02064] Fast inverse LU preconditioner based on the Sherman--Morrison formula

**Format :** Talk at Waseda University

**Author(s) :** José Mas (Universitat Politècnica de València)José Marín (Universitat Politècnica de València)Juana Cerdán (Universitat Politècnica de València)Rafael Bru (Universitat Politècnica de València)

**Abstract :** A fast version of an approximate inverse *LU* preconditioner to solve linear systems is constructed based on the Sherman--Morrison formula. A multiplicative decomposition of the approximate inverse of the coefficient matrix is obtained applying recursively the inversion formula. Moreover, this recursion can be expresed in a compact form which is used to compute the preconditioner.

The method is stable for nonsingular *M*-matrices and *H*-matrices.

Numerical results show that the new proposal is robust and competitive compared with other preconditioners.

## [01679] GMRES using pseudoinverse for range symmetric singular systems

**Format :** Talk at Waseda University

**Author(s) :** Kota Sugihara (National institute of informatics)Ken Hayami (Professor Emeritus, National Institute of Informatics/The Graduate University for Advanced Studies (SOKENDAI))

**Abstract :** For range symmetric singular linear systems, GMRES converges to the least squares solution in exact arithmetic. We derive necessary and sufficient conditions for GMRES to converge assuming exact arithmetic except for the computation of the elements of the Hessenberg matrix. In practice, GMRES may not converge due to numerical instability. Thus, we propose using the pseudoinverse for the solution of severely ill-conditioned Hessenberg systems. Numerical experiments indicate that the method is effective.

## [02051] Solving rank deficient mixed sparse-dense linear least-squares problems by updating preconditioned iterative methods

**Format :** Talk at Waseda University

**Author(s) :** Ning Zheng (The Institute of Statistical Mathematics)

**Abstract :** We consider the preconditioning of linear least squares problem when the large sparse coefficient matrix contains a few dense rows. Such mixed sparse dense least squares problem arises from many scientific practical problems. We propose preconditioned iterative methods for solving the problem when the sparse part is rank deficient and the whole system is rank deficient, respectively. Numerical experiments are presented to show the feasibility and efficiency of the proposed methods.

00810 (2/3) : 1D @E508 [Chair: Raymond Chan]

## [02061] Preconditioners based on random sampling for solving least squares problems

**Format :** Talk at Waseda University

**Author(s) :** Junfeng Yin (Tongji University)Yuxin Ye (Tongji University)Aqin Xiao (Tongji University)Nan Li (Tongji University)Ning Zheng (Tongji University)

**Abstract :** For the solution of large sparse least squares problems, preconditioned Krylov subspace methods are usually the fist choice and the preconditioners play the important roles in accelerating the convergence of the iteration. After the study on incomplete QR decomposition preconditioners based on Givens rotation, we proposed the preconditioners on random sampling and QR decomposition for solving least squares problems. Theoretical analysis and numerical experiments are presented to show the efficiency of the preconditioners, compared with the existing preconditioners.

## [01654] On Convergence Analysis of the Randomized Gauss-Seidel Method

**Format :** Online Talk on Zoom

**Author(s) :** Lu Wang (Hebei Normal University)

**Abstract :** The Gauss-Seidel and Kaczmarz methods are two classical iteration methods for solving systems of linear equations, which operate in column and row spaces, respectively. In this report, by utilizing the inner connections between these two methods and the convergence analysis of the randomized Kaczmarz method, we give a new upper bound for the convergence rate of the randomized Gauss-Seidel method. Moreover, these convergence results are extended to the more general extrapolated randomized Gauss-Seidel method.

## [01890] Condition numbers for the total least squares problems

**Format :** Online Talk on Zoom

**Author(s) :** Huaian Diao (Jilin University)

**Abstract :** The total least squares problems (TLS) is a generalization of the linear least squares problem and has many applications in linear system theory, computer vision, image reconstruction, system identification, speech and audio processing, modal and spectral analysis, etc. Perturbation analysis and algorithms for TLS have been studied extensively in the past decades. In this talk, I shall report our recent progresses on condition numbers for TLS.

## [02050] Quantum-inspired algorithm for truncated total least squares solution

**Format :** Talk at Waseda University

**Author(s) :** Yimin Wei (Fudan University)

**Abstract :** Compared with the ordinary least squares method, for total least squares (TLS) problem we take into account not only the observation errors, but also the errors in the measurement matrix, which is more realistic in practical applications. For the large-scale discrete ill-posed problem  $Ax \approx b$ , we introduce the quantum-inspired techniques to approximate the truncated total least squares (TTLS) solution.

00810 (3/3) : 1E @E508 [Chair: José Mas]

## [01317] Selecting Regularization Parameters for Nuclear Norm Type Minimization Problems

**Format :** Talk at Waseda University

**Author(s) :** Raymond Honfu Chan (City University of Hong Kong)Kexin Li (Hunan Normal University)Hongwei Li (Captial Normal University)Youwei Wen (Hunan Normal University)

**Abstract :** The reconstruction of low-rank matrix from its noisy observation is a constrained nuclear norm minimization problem, where the constraint bound  $\eta$  can be estimated from the noise variance. Its solution can be obtained by the singular value thresholding operator where the thresholding parameter  $\lambda$  is the same as the regularization parameter. We derive a closed-form solution for  $\lambda$  in terms of  $\eta$  which allows us to automatically choose  $\lambda$  by the discrepancy principle.

## [01895] A nonconvexly regularized least squares approach for sparsity aware estimation

**Format :** Talk at Waseda University

**Author(s) :** Masao Yamagishi (Tokyo Institute of Technology)Isao Yamada (Tokyo Institute of Technology)

**Abstract :** We present basic ideas and applications of a nonconvexly regularized least squares model ((\text{LiGME model})), which can achieve its overall convexity through strategic tuning of a matrix-valued parameter called the Generalized Moreau Enhancement ((\text{GME})) matrix. The LiGME model can exploit sparsity in a linearly transformed domain. Recent related advancements will also be introduced briefly.

## [02058] Separable Quaternion Matrix Factorization

**Author(s) :** Junjun Pan (The University of Hong Kong)Michael Ng (The University of Hong Kong)

**Abstract :** This presentation proposes a separable low-rank quaternion linear mixed model for polarized signals. The corresponding problem is called Separable Quaternion Matrix Factorization (SQMF). We discussed some properties of matrices that SQMF can decompose. We propose a heuristic algorithm called the quaternion successive projection algorithm to determine the source matrix. To compute the activation matrix, we use the block coordinate descent algorithm. Polarization and spectro-polarimetric images are tested to verify the model's effectiveness.

## [01543] GMRES methods for tomographic reconstruction with an unmatched back projector

**Format :** Talk at Waseda University

**Author(s) :** Ken Hayami (Professor Emeritus, National Institute of Informatics/The Graduate University for Advanced Studies (SOKENDAI))Per Christian Hansen (Technical University of Denmark)Keiichi Morikuni (University of Tsukuba)

**Abstract :** Unmatched pairs of forward and back projectors are common in X-ray CT computations due to the need for fast algorithms that best utilize the computer hardware. We propose using preconditioned GMRES, namely, AB-, BA- GMRES, to handle the unmatched normal equations. They are simple to implement and rely only on available forward and back projectors. Numerical experiments show that they exhibit a desired semi-convergence behavior and are suited for large-scale CT reconstruction problems with noisy data.

## [00814] Inverse Problems for Moving Targets

**Session Time & Room :**

00814 (1/2) : 1C (Aug.21, 13:20-15:00) @D405

00814 (2/2) : 1D (Aug.21, 15:30-17:10) @D405

**Type :** Proposal of Minisymposium

**Abstract :** The inverse problems of determining the trajectory of a moving target arise from many significant industrial, medical and military applications such as radar imaging, underwater sonar system , auto target recognition etc. There has been growing interest from the mathematical community, because the design of efficient and stable numerical schemes relies heavily on deep mathematical understandings. The purpose of this symposium is to bring together researchers in this area to discuss mathematical models and inverse problems (including uniqueness, stability and numerics) for identifying moving objects governed by time-dependent PDEs.

**Organizer(s) :** Guanghui Hu, Takashi Ohe, Jun Zou

**Classification :** 78A46, 65N21

**Minisymposium Program :**

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00814 (1/2) : 1C @D405 [Chair: Guanghui Hu]

## [03803] Direct reconstruction methods for moving sources in the wave equation

**Format :** Talk at Waseda University

**Author(s) :** Takashi Ohe (Okayama University of Science)

**Abstract :** In this talk, we consider the reconstruction problem of moving wave sources under different observation conditions; one is observations on the boundary, and the other is observations on a small number of points. For each observation condition, we propose a direct reconstruction procedure for the parameters of moving wave sources. We also discuss the common and different issues between reconstruction procedures.

## [03831] An inverse problem in mean field game from partial boundary measurement

**Format :** Online Talk on Zoom

**Author(s) :** Yat Tin Chow (University of California, Riverside)Samy Wu Fung (Colorado School of Mines)Siting Liu (University of California, Los Angeles)Levon Nurbekyan (University of California, Los Angeles)Stanley Osher (University of California, Los Angeles)

**Abstract :** In this work, we consider a novel inverse problem in mean-field games (MFG). We aim to recover the MFG model parameters that govern the underlying interactions among the population based on a limited set of noisy partial observations of the population dynamics under the limited aperture. Due to its severe ill-posedness, obtaining a good quality reconstruction is very difficult. Nonetheless, it is vital to recover the model parameters stably and efficiently in order to uncover the underlying causes for population dynamics for practical needs.

Our work focuses on the simultaneous recovery of running cost and interaction energy in the MFG equations

from a finite number of boundary measurements of population profile and boundary movement. To achieve this goal, we formalize the inverse problem as a constrained optimization problem of a least squares residual functional under suitable norms with L1 regularization. We then develop a fast and robust operator splitting algorithm to solve the optimization using techniques including harmonic extensions, three-operator splitting scheme, and primal-dual hybrid gradient method. Numerical experiments illustrate the effectiveness and robustness of the algorithm.

This is a joint work with Samy W. Fung (Colorado School of Mines), Siting Liu (UCLA), Levon Nurbekyan (UCLA), and Stanley J. Osher (UCLA)

## **[02996] Factorization method for recovering moving objects with dynamic near-field data**

**Format :** Online Talk on Zoom

**Author(s) :** Hongxia Guo (Nankai University)

**Abstract :** In this talk, I will present the factorization method for recovering the trajectory of a moving point source from multi-frequency data with one or sparse dynamic near-field observation points . The observable and non-observable points in the near field region are introduced. At an observable point, it is verified that the smallest annular containing the trajectory and centered at the observable point can be imaged, provided the orbit function possessing a certain property.

## **[04620] Imaging a moving point source from multi-frequency data measured at one and sparse observation directions (part I): far-field case**

**Format :** Online Talk on Zoom

**Author(s) :** Hongxia Guo (Nankai University)Guanghui Hu (Nankai University, Tianjin, China)Guanqiu Ma (Nankai University)

**Abstract :** We propose a multi-frequency algorithm for recovering partial information on the trajectory of a moving point source from one and sparse far-field observation directions in the frequency domain. The starting and terminal time points of the moving source are both supposed to be known.

We introduce the concept of observable directions (angles) in the far-field region and derive all observable directions (angles) for straight and circular motions. The existence of non-observable directions makes this paper much different from inverse stationary source problems.

At an observable direction, it is verified that the smallest strip containing the trajectory and perpendicular to the direction can be imaged, provided the angle between the observation direction and the velocity vector of the moving source lies in \$

**[0,\pi/2]\$.**

If otherwise, one can only expect to recover a strip thinner than this smallest strip for straight and circular motions. The far-field data measured at sparse observable directions can be used to recover the  $\Theta$ -convex domain of the trajectory. Both two- and three-dimensional numerical examples are implemented to show effectiveness and feasibility of the approach.

00814 (2/2) : 1D @D405

## **[00815] Recent trends in continuous optimization**

**Session Time & Room :**

00815 (1/4) : 1C (Aug.21, 13:20-15:00) @A502

00815 (2/4) : 1D (Aug.21, 15:30-17:10) @A502

00815 (3/4) : 1E (Aug.21, 17:40-19:20) @A502

00815 (4/4) : 2C (Aug.22, 13:20-15:00) @A502

**Type :** Proposal of Minisymposium

**Abstract :** Continuous optimization is a branch of optimization with applications in many fields. In view of their usefulness, in this minisymposium we will focus on: (i) nonlinear programming, where an objective function is minimized or maximized while satisfying some constraints; (ii) multiobjective optimization, where multiple objective functions are considered; and (iii) conic optimization, which deals with more general conic constraints. The goal of this minisymposium is to present some recent developments on those topics. In particular, proposals of efficient algorithms, advanced theoretical results and applications in machine learning will be discussed.

**Organizer(s) :** Yasushi Narushima, Ellen H. Fukuda, Bruno F. Lourenço

**Classification :** 90Cxx, 90C30, 90C25, 90C06, 90C29

**Minisymposium Program :**

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00815 (1/4) : 1C @A502 [Chair: Ellen Hidemi Fukuda]

## [03738] Recent developments in multiobjective fast iterative shrinkage-thresholding algorithms

**Format :** Talk at Waseda University

**Author(s) :** Ellen Hidemi Fukuda (Kyoto University)

**Abstract :** In this talk, we will present an overview of multiobjective proximal gradient methods, that solve problems of the type  $\min f(x) + g(x)$ , where  $f: \mathbb{R}^n \rightarrow \mathbb{R}^m$  is continuously differentiable and  $g: \mathbb{R}^n \rightarrow (\mathbb{R} \cup \{+\infty\})^m$  is closed, proper and convex. We will also discuss their accelerated versions, including the multiobjective fast iterative shrinkage-thresholding algorithm (FISTA), monotone FISTA, and restarting FISTA. We will show the associated convergence results and some numerical experiments.

## [04395] Adaptive Gradient-Based Method for Convex Optimization Problems Under Error Bounds

**Format :** Talk at Waseda University

**Author(s) :** Masaru Ito (Nihon University)

**Abstract :** First-order methods for smooth convex optimization problems is a fundamental methodology for large-scale optimization arising in machine learning. We present an adaptive first-order method to find an approximate solution in terms of small gradient norm that does not require the problem dependent parameters and automatically accelerates under error bound condition like strong convexity. The iteration complexity to find an approximate solution is shown to be optimal.

## [03739] Accelerated distributed proximal conjugate gradient methods for multi-agent constrained optimization problems

**Format :** Talk at Waseda University

**Author(s) :** Gebrie Anteneh Getachew (Debre Berhan University)Stefan Volkwein (University of Konstanz)

**Abstract :** We introduce two new classes of accelerated distributed proximal conjugate gradient algorithms for multi-agent constrained optimization problems; given as minimization of a function decomposed as a sum of M number of smooth and M number of non-smooth functions over the common fixed points of M number of nonlinear mappings. Exploiting the special properties of the cost component function of the objective function and the nonlinear mapping of the constraint problem of each agent, a new inertial accelerated incremental and parallel computing distributed algorithms will be presented based on the combinations of computations of proximal, conjugate gradient and Halpern methods. Some numerical experiments and comparisons are given to illustrate our results.

## [03850] Extensions of Constant Rank Qualification Constraints condition to Nonlinear Conic Programming

**Format :** Talk at Waseda University

**Author(s) :** Hector Ramirez (Universidad de Chile)

**Abstract :** We present new constraint qualification conditions for nonlinear conic programming that extend some of the constant rank-type conditions from nonlinear programming. Specifically, we propose a general and geometric approach, based on the study of the faces of the cone, for defining a new extension of this condition to the conic context. We then compare these new conditions with some of the existing ones, including the nondegeneracy condition, Robinson's constraint qualification, and the metric subregularity constraint qualification. The main advantage of the latter is that we are able to recast the strong second-order properties of the part\_2

constant rank condition in a conic context. In particular, we obtain a second-order necessary optimality condition that is stronger than the classical one obtained under Robinson's constraint qualification, in the sense that it holds for every Lagrange multiplier, even though our condition is independent of Robinson's condition.

00815 (2/4) : 1D @A502 [Chair: Pierre-Louis Poirion]

### **[03316] Derivative-free Low Order-Value Optimization**

**Format :** Online Talk on Zoom

**Author(s) :** Anderson Ervino Schwertner (State University of Maringá)Francisco Nogueira Calmon Sobral (State University of Maringá)

**Abstract :** The Low Order-Value Optimization (LOVO) problem seeks to minimize the minimum among a finite number of function values within a feasible set and has several applications, such as protein alignment and portfolio optimization, among others. In this work, we are interested in the constrained black-box LOVO problem, whose feasible set is convex, closed, and nonempty. We developed and implemented a derivative-free trust-region algorithm, and established global convergence and worst-case complexity results.

### **[04101] A Stochastic Variance Reduced Gradient using Second Order Information**

**Format :** Talk at Waseda University

**Author(s) :** Hardik Tankaria (Kyoto University)Nobuo Yamashita (Kyoto University)

**Abstract :** In this talk, we consider to improve the stochastic variance reduced gradient (SVRG) method via incorporating the curvature information of the objective function. We propose to reduce the variance of stochastic gradients using the computationally efficient method of second order approximation by incorporating it into the SVRG. We also incorporate a (Barzilai-Borwein) BB-step size as its variant. We show linear convergence for not only the proposed method but also for the other existing SVRG variants that use second-order information as a variance reduction. We show the numerical experiments on the benchmark datasets and demonstrate the comparison of proposed methods with existing variance reduced methods.

### **[03875] Post-Processing with Projection and Rescaling Algorithm for Symmetric Cone Programs**

**Format :** Talk at Waseda University

**Author(s) :** Shinichi Kanoh (University of Tsukuba)Akiko Yoshise (University of Tsukuba)

**Abstract :** We propose a post-processing algorithm for symmetric cone programs based on the Projection and Rescaling Algorithm (PRA). Our algorithm is devised to return a more accurate solution using the output solution from MOSEK solver and the PRA proposed by Kanoh & Yoshise (2021). Numerical experiments with SDPLIB instances show that our algorithm outputs a solution with a very small value of DIMACS error compared to the solution that MOSEK solver returned.

### **[04338] Random Subsapce Newton method for unconstrained non-convex optimization**

**Format :** Talk at Waseda University

**Author(s) :** Pierre-Louis Poirion (RIKEN -AIP)

**Abstract :** In this talk, we present a randomized subspace regularized Newton method for a non-convex function. We will be interested in particular to the local convergence rate of the method.

00815 (3/4) : 1E @A502 [Chair: Yasushi Narushima]

### **[01619] Generalized Levenberg-Marquardt method with oracle complexity bound and local convergence**

**Format :** Talk at Waseda University

**Author(s) :** Naoki Marumo (University of Tokyo)Akiko Takeda (University of Tokyo)Takayuki Okuno (Seikei University)

**Abstract :** The generalized Levenberg–Marquardt, abbreviated as LM, method has been developed for minimizing the sum of a possibly nonsmooth convex function and a smooth composite function. In this talk, we propose a new

generalized LM method with three theoretical guarantees: iteration complexity bound, oracle complexity bound, and local convergence under a Holderian growth condition. These theoretical guarantees are achieved by use of an accelerated gradient method for solving convex subproblems.

### **[04603] Line search methods for nonconvex optimization in deep learning**

**Format :** Online Talk on Zoom

**Author(s) :** Yuki Tsukada (Meiji University)Hideaki Iiduka (Meiji University)

**Abstract :** Stochastic gradient descent (SGD) using line search methods achieves high accuracies for several classification tasks in deep learning. Moreover, it can find optimal parameters for deep neural network models by using nonconvex optimization. This talk experimentally investigates the convergence speed of SGD using line search methods with several batch sizes. Our results indicate that the smaller the batch size is, the smaller the stochastic first-order oracle complexity becomes.

### **[01615] Proximal structured quasi-Newton method for nonlinear least squares with nonsmooth regularizer**

**Format :** Talk at Waseda University

**Author(s) :** Shummin Nakayama (The University of Electro-Communications)Yasushi Narushima (Keio University)Hiroshi Yabe (Tokyo University of Science)

**Abstract :** We consider composite minimization problems whose objective function is the sum of a nonlinear least squares formed smooth function and a nonsmooth regularizer. Structured quasi-Newton methods are efficient for solving nonlinear least squares problems and proximal Newton-type methods are efficient for composite minimization problems. In this talk, combining the above two methods, we propose a proximal structured quasi-Newton-type method. Finally, we present some numerical experiments to investigate the efficiency of the proposed method.

### **[03538] Newton-type proximal gradient method for multi-objective optimization with composite D.C. functions**

**Format :** Talk at Waseda University

**Author(s) :** Yasushi Narushima (Keio University)Antoine J.V. Vadès (Keio University)Hiroshi Ben (Keio University)

**Abstract :** In this talk, we propose a Newton-type proximal gradient method for multi-objective optimization whose objective functions are the sum of a continuously differentiable function and a Difference of Convex (D.C.) function. The proposed method is an extension of Newton-type proximal gradient methods for single-objective optimization. We give an algorithm of the proposed method with the Armijo-type line search and show its global convergence. Finally, we present some numerical results for comparison with the existing methods.

00815 (4/4) : 2C @A502 [Chair: Bruno F. Lourenço]

### **[04582] Sharp convex exact penalty formulations in statistical signal recovery**

**Format :** Talk at Waseda University

**Author(s) :** Alex Liheng Wang (Purdue University)Lijun Ding (University of Wisconsin Madison)

**Abstract :** This talk presents a sample complexity vs. conditioning tradeoff in signal recovery problems including sparse recovery, low-rank matrix sensing, and phase retrieval. We introduce condition numbers related to the "sharpness" of these problems and show that they can be used to control the accuracy of the recovery procedure in the presence of noise and the convergence rates of a new first-order method. These condition numbers approach constants a small factor above the statistical thresholds.

### **[02314] Accelerating nuclear-norm regularized low-rank matrix optimization through Burer-Monteiro decomposition**

**Format :** Talk at Waseda University

**Author(s) :** Ching-pei Lee (Institute of Statistical Mathematics)Ling Liang (National University of Singapore)Tianyun Tang (National University of Singapore)Kim-Chuan Toh (National University of Singapore)

**Abstract :** This work proposes a rapid algorithm, BM-Global, for nuclear-norm-regularized convex and low-rank matrix optimization problems. BM-Global efficiently decreases the objective value via low-cost steps leveraging the

nonconvex but smooth Burer-Monteiro (BM) decomposition, while effectively escapes saddle points and spurious local minima ubiquitous in the BM form to obtain guarantees of fast convergence rates to the global optima of the original nuclear-norm-regularized problem through aperiodic inexact proximal gradient steps on it. The proposed approach adaptively adjusts the rank for the BM decomposition and can provably identify an optimal rank for the BM decomposition problem automatically in the course of optimization through tools of manifold identification. BM-Global hence also spends significantly less time on parameter tuning than existing matrix-factorization methods, which require an exhaustive search for finding this optimal rank. Extensive experiments on real-world large-scale problems of recommendation systems, regularized kernel estimation, and molecular conformation confirm that BM-Global can indeed effectively escapes spurious local minima at which existing BM approaches are stuck, and is a magnitude faster than state-of-the-art algorithms for low-rank matrix optimization problems involving a nuclear-norm regularizer.

## [05168] The Goemans and Williamson Algorithm Extended to Fractional Cut Covering

**Format :** Talk at Waseda University

**Author(s) :** Nathan Benedetto Proen  a (University of Waterloo)Marcel K. de Carli Silva (University of S  o Paulo)Cristiane Sato (Federal University of ABC Region)Levent Tun  el (University of Waterloo)

**Abstract :** The fractional cut-covering number is the optimal value of a linear programming relaxation for the problem of covering each edge by a set of cuts.

By exploiting the relationship of this problem with the maximum cut problem, we obtain a primal-dual extension to the celebrated work of Goemans and Williamson, including an approximation algorithm and new optimality certificates.

## [01270] Solving graph equipartition SDPs on an algebraic variety

**Format :** Talk at Waseda University

**Author(s) :** Tianyun Tang (National University of Singapore)Kim-Chuan Toh (National University of Singapore)

**Abstract :** In this talk, we focus on using the Burer-Monteiro method to solve the graph equipartition SDP. The constraints of the low rank SDP problem is an algebraic variety with conducive geometric properties which we analyse. This allows us to develop an algorithm based on Riemannian optimization that can escape from a non-optimal singular point. Numerical experiments are conducted to verify the efficiency of our algorithm.

## [00819] Secure Computing: Maintaining Personal Privacy while Analyzing Data

**Session Time & Room :** 3D (Aug.23, 15:30-17:10) @E804

**Type :** Proposal of Industrial Minisymposium

**Abstract :** The proliferation of IoT machine and sensor devices are major contributors to the surge in production and storage of mostly private, sensitive data. Deloitte projects, "by 2025 our global volume will reach 175 zeta bytes" ([www2.deloitte.com/cy/en/pages/technology/articles/data-grown-big-value.html](http://www2.deloitte.com/cy/en/pages/technology/articles/data-grown-big-value.html)). Many data owners seek to analyze the data to uncover insights and improve their decision-making processes. However, compliance with privacy regulations and the threat of cyberattacks pose heretofore unknown challenges. Approaches to address this issue, collectively known as secure computing, include: privacy-preserving data analysis, differential privacy, federated learning, multi-party computation, and homomorphic encryption. This mini-symposium seeks to gather practitioners/specialists for active debate and dialog.

**Organizer(s) :** Mei Kobayashi

**Classification :** 68M25, Computer security, Privacy of data, Data encryption (aspects in computer science), Artificial neural networks and deep learning

**Minisymposium Program :**

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00819 (1/1) : 3D @E804 [Chair: Mei Kobayashi]

## [04041] Construction of Differentially Private Summary with Homomorphic Encryption

**Format :** Talk at Waseda University

**Author(s) :** HAYATO YAMANA (Waseda University)Shojiro USHIYAMA (Waseda University)Tsubasa TAKAHASHI (LINE Corp.)

**Abstract :** A differentially private summary for range queries is constructed using homomorphic encryption to hide the raw data from the computation server. To shorten the processing time, we proposed a new method to merge adjacent close values in the histogram if the difference between the adjacent data is small. Then, we confirmed that the accuracy of the proposed method was equivalent to a state-of-the-art algorithm and the processing time is  $O(n)$ .

## [04961] Federated Learning with Differential Privacy and Secure Computing

**Format :** Talk at Waseda University

**Author(s) :** Tsubasa Takahashi (LINE Corporation)

**Abstract :** Improving user experience while respecting user privacy is important nowadays. Last year we released federated learning in LINE messenger's keyboard area to make users sticker selection easier and more personalized while preserving user privacy. Our FL also employs Differential Privacy (DP) to make exploiting user privacy more difficult. This talk presents our FL+DP, and recent advancement of privacy amplification with secure computing.

## [05348] Network Security and Analytics for Reliability

**Format :** Talk at Waseda University

**Author(s) :** Yukio Uematsu (Tokyo University of Science/Nokia)

**Abstract :** In recent years, a vast number of IoT devices have been connected to the cloud through mobile networks. This talk will address two fundamental issues, namely security and data reliability, in the context of mobile network data analytics. We will present some use cases for data management that combine edge and cloud computing while ensuring data reliability.

# [00825] Numerical Time Integration Algorithms and Software for Machine Learning

**Session Time & Room :** 4E (Aug.24, 17:40-19:20) @E508

**Type :** Proposal of Minisymposium

**Abstract :** Decades of research and development in numerical time integration algorithms and software has been focused on solving time-dependent differential equations that arise from mathematical models of physical phenomena. Recently, a clear nexus between time integration and machine learning (ML) has been established, giving rise to many new opportunities for novel time-integration algorithm research and software development. The goal of this minisymposium is to shine a light on the ML application area by featuring talks that demonstrate numerical time integration algorithms and software benefiting ML, or discuss how they can be geared towards ML. Prepared by LLNL under Contract DE-AC52-07NA27344. LLNL-ABS-843420.

**Organizer(s) :** Cody Balos, Richard Archibald

**Classification :** 65L99, 65M99, 68T07, 65C99

**Minisymposium Program :**

00825 (1/1) : 4E @E508 [Chair: Cody Balos]

## [04991] The Roles of Numerical Time Integration Algorithms and Software in the Machine Learning Revolution

**Format :** Talk at Waseda University

**Author(s) :** Cody Balos (Lawrence Livermore National Lab)

**Abstract :** Recently large language models like OpenAI's ChatGPT have sparked mainstream discussion of Artificial Intelligence and Machine Learning. Meanwhile, in the scientific community there has been an increased interest in Scientific Machine Learning (SciML) and a substantial shift in funding opportunities towards work with at least some ML component. In this talk, I will explore some examples of how numerical time integration algorithms and software, which have been critical to scientific computing for decades, are playing a part in this ML revolution. As part of this exploration, I will also discuss what we are doing in the SUNDIALS time integration library to enable ML applications. LLNL-ABS-847841.

## [03318] TransNet: Transferable Neural Networks for Partial Differential Equations

**Format :** Online Talk on Zoom

**Author(s) :** Zezhong Zhang (Florida State University)Feng Bao (Florida State University)Lili Ju (University of South Carolina)Guannan Zhang (Oak Ridge National Laboratory)

**Abstract :** Transfer learning for partial differential equations (PDEs) is to develop a pre-trained neural network that can be used to solve a wide class of PDEs. Existing transfer learning approaches require much information of the target PDEs such as its formulation and/or data of its solution for pre-training. In this work, we propose to construct transferable neural feature spaces from purely function approximation perspectives without using PDE information. The construction of the feature space involves re-parameterization of the hidden neurons and uses auxiliary functions to tune the resulting feature space. Theoretical analysis shows the high quality of the produced feature space, i.e., uniformly distributed neurons. Extensive numerical experiments verify the outstanding performance of our method, including significantly improved transferability, e.g., using the same feature space for various PDEs with different domains and boundary conditions, and the superior accuracy, e.g., several orders of magnitude smaller mean squared error than the state of the art methods.

## [04020] Dissipative residual layers for unsupervised implicit parameterization of data manifolds

**Format :** Online Talk on Zoom

**Author(s) :** Viktor Reshniak (Oak Ridge National Laboratory)

**Abstract :** We propose an unsupervised technique for implicit parameterization of data manifolds. In our approach, the data is assumed to belong to a lower dimensional manifold in a higher dimensional space, and the data points are viewed as the endpoints of the trajectories originating outside the manifold. Under this assumption, the data manifold is an attractive manifold of a dynamical system to be estimated. We parameterize such a dynamical system with a residual neural network and propose a spectral localization technique to ensure it is locally attractive in the vicinity of data. We also present initialization and discuss the regularization of the proposed residual layers that we call dissipative bottlenecks.

## [03338] Improved Parallelism and Memory Performance for Differentiating Stiff Differential Equations

**Format :** Online Talk on Zoom

**Author(s) :** Christopher Vincent Rackauckas (Julia Hub, Pumas-AI, MIT)

**Abstract :** Previous work demonstrated trade-offs in performance, numerical stability, and memory usage for ODE solving and differentiation of solutions. Our new time stepping methods expose more parallelism is shown to accelerate small ODE solves, while new GPU-based ODE solvers demonstrate a 10x performance improvement over Jax and PyTorch-based solvers. New adjoint methods achieve linear cost scaling with respect to parameters in stiff ODEs, as opposed to the cubic of Jax/PyTorch, while limiting the memory scaling.

# [00827] Stochastic Rounding for Reduced-Precision Arithmetic in Scientific Computing

**Session Time & Room :** 2E (Aug.22, 17:40-19:20) @E709

**Type :** Proposal of Minisymposium

**Abstract :** The comeback that stochastic rounding has made in the last few years can be attributed to the availability of hardware implementing low-precision floating-point arithmetic, as well as to the recognition that, in some applications, this rounding mode can control the growth of rounding errors better than commonly used alternatives. Research has focused not only on obtaining efficient hardware and software implementations, but also on understanding the numerical properties of algorithms that replace round-to-nearest with stochastic rounding. In this minisymposium, we will have an opportunity to learn about recent advances in both directions.

**Organizer(s) :** Massimiliano Fasi, Mantas Mikaitis

**Classification :** 65Y04, 65Y10, 68M07, 68Q87, Computer arithmetic, Stochastic Rounding

**Minisymposium Program :**

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00827 (1/1) : 2E @E709 [Chair: Xiaobo Liu]

## [03817] Implementation of Stochastic Rounding

**Format :** Online Talk on Zoom

**Author(s) :** Mantas Mikaitis (University of Leeds)

**Abstract :** In this talk we will review the latest developments in implementing stochastic rounding. We will first revisit the current methods of implementing stochastic rounding in hardware and software packages, such as CPFloat and MATLAB chop. We will present the main challenges and open problems, such as the reproducibility and precision of pseudo-random numbers. We will also review the commercial hardware that currently includes stochastic rounding, such as Graphcore IPU, Amazon Trainium, and Tesla Dojo devices. Finally, we will outline the list of features required for stochastic rounding to be standardized.

## [04133] Software Simulation of Stochastic Rounding

**Format :** Online Talk on Zoom

**Author(s) :** Massimiliano Fasi (Durham University)Mantas Mikaitis (University of Leeds)

**Abstract :** Implementing a stochastically rounded mathematical function requires three steps: 1) evaluating the function using a high-precision floating-point arithmetic; 2) drawing a pseudo-random number from some uniform distribution; and 3) rounding the high-precision result to the target precision. We describe how stochastic rounding can be performed using only integer arithmetic and bit-level operations, and we summarize the major challenges and open questions surrounding the implementation of this rounding mode.

## [04508] Bounds on Non-linear Errors for Variance Computation with Stochastic Rounding

**Format :** Talk at Waseda University

**Author(s) :** El-Mehdi El Arar (Paris-Saclay University-UVSQ- LI-PaRAD )Devan Sohier (Paris-Saclay University-UVSQ- LI-PaRAD )Pablo de Oliveira Castro (Paris-Saclay University-UVSQ- LI-PaRAD )Eric Petit (Intel Corp)

**Abstract :** This work's main objective is to investigate non-linear errors and pairwise summation using stochastic rounding (SR) in variance computation algorithms. We estimate the forward error of computations under SR through two methods: 1 a bound of the variance and Bienaym  -Chebyshev inequality, 2 martingales and Azuma-Hoeffding inequality. We examine two algorithms, "textbook" and "two-pass", both with non-linear errors. We show that they have probabilistic bounds under SR in  $O(\sqrt{n}u)$  instead of  $nu$  for the deterministic bounds.

## [04837] Trace estimation via asynchronous stochastic rounding

**Format :** Online Talk on Zoom

**Author(s) :** Lior Horesh (IBM T. J. Watson Research Center)Vasileios Kalantzis (IBM T. J. Watson Research Center)Georgios Kollias (IBM T. J. Watson Research Center)Shashanka Ubaru (IBM T. J. Watson Research Center)Chai Wah Wu (IBM T. J. Watson Research Center)

**Abstract :** We present a framework of randomized algorithms that include stochastic rounding and asynchronous updates and apply it to randomized linear algebra algorithms. In particular, we analyze an application to trace estimation and show its efficacy on various real-world datasets.

# [00831] Randomization for Simplified Machine Learning: Random Features and Reservoir Computers

**Session Time & Room :**

00831 (1/3) : 2C (Aug.22, 13:20-15:00) @E507

00831 (2/3) : 2D (Aug.22, 15:30-17:10) @E507

00831 (3/3) : 2E (Aug.22, 17:40-19:20) @E507

**Type :** Proposal of Minisymposium

**Abstract :** Training neural networks remains challenging for complex or recurrent architectures. The random feature approach side steps training deep layers by sampling random weights and fitting only the final output layer to data with linear least squares. When applied to recurrent networks, this is called a reservoir computer. These methods can approximate functions, operators, and dynamical systems. This minisymposium seeks to unify knowledge and experiences of both communities on topics of 1) scaling to high-dimensional large-volume data, 2) hyperparameter learning, 3) performance evaluation and comparison, and 4) theoretical understanding of features and reservoirs.

**Organizer(s) :** Oliver Dunbar, Georg Gottwald, Matthew Levine, Nicholas Nelsen

**Classification :** 65D15, 65C20, 68T05, 60G15, 62M45, Machine Learning

**Minisymposium Program :**

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00831 (1/3) : 2C @E507 [Chair: Oliver Dunbar]

## [02997] Scalable Gaussian Process Regression with Quadrature-based Features

**Format :** Talk at Waseda University

**Author(s) :** Paz Fink Shustein (Tel Aviv University)

**Abstract :** Gaussian processes provide a powerful probabilistic kernel learning framework, which allows high-quality nonparametric learning via methods such as Gaussian process regression. Nevertheless, its learning phase requires unrealistic massive computations for large datasets. In this talk, we present a quadrature-based approach for scaling up Gaussian process regression via a low-rank approximation of the kernel matrix. The low-rank structure is utilized to achieve effective hyperparameter learning, training, and prediction. Our Gauss-Legendre features method is inspired by the well-known random Fourier features approach, which also builds low-rank approximations via numerical integration. However, our method is capable of generating high-quality kernel approximation using a number of features that is poly-logarithmic in the number of training points, while similar guarantees will require an amount that is at the very least linear in the number of training points when using random Fourier features. The utility of our method for learning with low-dimensional datasets is demonstrated using numerical experiments.

## [03226] Advances in Time Series Analysis With Reservoir Computing

**Format :** Talk at Waseda University

**Author(s) :** Braden John Thorne (University of Western Australia) Michael Small (University of Western Australia) Débora Cristina Corrêa (University of Western Australia) Ayham Zaitouny (University of Doha for Science and Technology)

**Abstract :** Reservoir computers have proven to be powerful embedding machines for dynamical systems. However, bridging the gap from their machine learning origins to time series analysis is still relatively new, with great potential for novel discoveries. In this talk, we will outline what reservoir time series analysis is and why one should care about it amidst the ecosystem of other embedding-based techniques. We will then present some use cases and applications to motivate future work.

## [03272] Error analysis of random feature neural networks for Black-Scholes-type PDEs

**Format :** Online Talk on Zoom

**Author(s) :** Lukas Gonon (Imperial College London)

**Abstract :** We mathematically analyse the learning performance of random feature neural networks for learning solutions to a class of PDEs which includes the Black-Scholes PDE as special case. In contrast to other existing mathematical results on neural network-based PDE-learning, in our context it is possible to obtain a full error analysis addressing all error components (approximation, generalization and optimization) with the derived bounds (convergence rates and constants) not suffering from the curse of dimensionality.

## [04091] Theoretical advances for learning functions and operators with random features

**Format :** Talk at Waseda University

**Author(s) :** Nicholas H. Nelsen (California Institute of Technology)

**Abstract :** This talk provides a complete error analysis of operator learning with random features (RF). The theoretical results are developed in a fully general infinite-dimensional input-output setting. The highlights include strong consistency of RF estimators under model misspecification and minimax optimal convergence rates. This work also contributes theory for rigorous uncertainty quantification by establishing (i) new pointwise error bounds for vector-valued Gaussian process (GP) regression and (ii) strong consistency of RF estimators of GPs.

00831 (2/3) : 2D @E507 [Chair: Matthew Levine]

## [04530] Photonic reservoir computing with small networks

**Format :** Online Talk on Zoom

**Author(s) :** Joseph David Hart (US Naval Research Laboratory) Thomas Carroll (US Naval Research Laboratory) Francesco Sorrentino (University of New Mexico) Joel Q Grim (US Naval Research Laboratory) Allan Bracker (US Naval Research Laboratory)

**Abstract :** The model-free training permitted by reservoir computing makes it particularly attractive for implementation in analog physical hardware, which can offer significant improvements in speed and power requirements over digital hardware. In many cases, however, it can be difficult or undesirable to build a large, tunable analog network. In this talk, we will present recent results using photonic analog hardware to implement reservoir computers made up of small networks.

## [04854] Latent GP-ODEs with Informative Priors

**Format :** Online Talk on Zoom

**Author(s) :** Ilze Amanda Auzina (University of Amsterdam) Cagatay Yildiz (University of Tuebingen) Efstratios Gavves (University of Amsterdam)

**Abstract :** We propose a novel framework by combining a generative and a Bayesian nonparametric model which learns a physically meaningful latent representation and solves an ODE system in latent space. The model is able to account for uncertainty as well as to be constrained with informative physical priors. The method demonstrates its ability to learn dynamics from high dimensional data and we obtain state-of-the-art performance compared to earlier nonparametric ODE models on dynamic forecasting.

## [04314] A Framework for Hyperparameter Optimization for Randomized Machine Learning

**Format :** Talk at Waseda University

**Author(s) :** Oliver Dunbar (Division of Geological and Planetary Sciences, California Institute of Technology)Nicholas Nelsen (California Institute of Technology)Maya Mutic (Princeton University)

**Abstract :** Randomization can be used to replace layers of neural networks or kernel matrices of Gaussian processes. This approach accelerates numerical methods and converts training to a least-squares problem. In practice however, necessary hyperparameter optimization becomes more challenging, as optimization objective functions are non-deterministic. In the context of the random features, we present a framework and algorithm based on the ensemble Kalman filter, that can automate this optimization, and demonstrate practical performance through illustrative examples.

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00831 (3/3) : 2E @E507 [Chair: Georg Gottwald]

## [04861] Next-Generation Reservoir Computing, and On Explaining the Surprising Success of a Random Neural Network for Forecasting Chaos

**Format :** Online Talk on Zoom

**Author(s) :** Erik Matthew Boltt (Clarkson University)

**Abstract :** Machine learning is widely popular and successful, including for data-driven science, especially for forecasting complex dynamical systems. Reservoir computers (RC) have emerged as random neural networks, for simplicity and computational advantage, where only read-out weights are trained. That it is cheap is clear, but that it works at all is perhaps a surprise, which we explain here. Furthermore our discussion leads to a new, equivalent even simpler variant we call, next generation reservoir computing, NG-RC.

## [05356] Minimax optimal inference of inhomogeneous diffusions

**Format :** Online Talk on Zoom

**Author(s) :** Grant Rotskoff (Stanford University)

**Abstract :** Inferring a diffusion equation from discretely-observed measurements is a statistical challenge of significant importance in a variety of fields, from single-molecule tracking in biophysical systems to modeling financial instruments. Assuming that the underlying dynamical process obeys a  $d$ -dimensional stochastic differential equation of the form

$$d\mathbf{x}_t = \mathbf{b}(\mathbf{x}_t)dt + \Sigma(\mathbf{x}_t)d\mathbf{w}_t,$$

we show that no diffusion estimator using  $N$  discretely sampled data points converges faster than  $N^{-\frac{2s+2}{2s+2+d}}$  when the drift  $\mathbf{b}$  and diffusion tensor  $D = \Sigma\Sigma^T$  are  $s$  and  $s + 1$ -Hölder continuous, respectively. We further propose neural network estimators for both  $D$  and  $\mathbf{b}$ , establish convergence guarantees, and show that the estimators achieve a nearly optimal rate for correlated data.

## [05361] Nonlinear Time Series Analysis and Data Driven Forecasting: Regional Weather Prediction & Earth's Geodynamo

**Format :** Online Talk on Zoom

**Author(s) :** Luke Fairbanks (UCSD)Ashley Thorshov (UCSD)

**Abstract :** Amongst the zoo of complex systems analysis frameworks and methods exist some which leverage tools from mathematics and physics with machine learning to attempt a more interpretable and possibly better results with respect to time series prediction of said systems. Our work in the domains of weather prediction and the geodynamo is a model for the interdisciplinary union between experimentalists, theorists, and computational researchers such as ourselves in the pursuit of complex system algorithmic synchronization.

## [04474] Random Features for Epidemic Prediction

**Format :** Online Talk on Zoom

**Author(s) :** Esha Saha (University of Waterloo)Lam Ho (Dalhousie University )Giang Tran (University of Waterloo)

**Abstract :** Predicting the evolution of diseases is challenging. Compartmental models stratify the population into compartments and model the dynamics using dynamical systems. These predefined systems may not capture the true dynamics of the epidemic due to the complexity variable interactions. We propose Sparsity and Delay

Embedding based Forecasting (SPADE4) for predicting epidemics for predicting the future trajectory of a variable without the knowledge of the underlying system using random features and Takens' delay embedding theorem.

## [00837] Particle Methods for Bayesian Inference

### **Session Time & Room :**

00837 (1/3) : 4C (Aug.24, 13:20-15:00) @E709

00837 (2/3) : 4D (Aug.24, 15:30-17:10) @E709

00837 (3/3) : 4E (Aug.24, 17:40-19:20) @E709

**Type :** Proposal of Minisymposium

**Abstract :** Particle methods have become a popular method for sampling, optimization, inversion, and filtering. Moreover gradient-free versions of particle systems may implicitly carry gradient information that can be leveraged for better performance. In this minisymposium we bring together experts in Ensemble Kalman filtering, Ensemble Kalman inversion, and Ensemble Kalman sampling as well as other particle-based algorithms like Consensus-based optimization, Affine invariant Langevin dynamics, Stein Variational Gradient Descent and collect recent advances based on homotopy approaches, ensemble enrichment, Wasserstein gradient flows and discrepancy flows.

**Organizer(s) :** Robert Gruhlke, Johannes Hertwich, David Sommer, Philipp Wacker

**Classification :** 65N21, 62F15, 65N75, 65C30, 35Q84

### **Minisymposium Program :**

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00837 (1/3) : 4C @E709 [Chair: Johannes Hertwich]

## [05135] Improving Ensemble Kalman Filter performance by adaptively controlling the ensemble

**Format :** Talk at Waseda University

**Author(s) :** Ruben Harris (FU Berlin) Claudia Schillings (FU Berlin)

**Abstract :** Efficient strategies to improve the performance of the Ensemble Kalman Inversion by adaptively controlling the ensemble.

Due to their low computational costs and straightforward implementation, filtering methods such as the Ensemble Kalman Filter have become very popular for inverse problems over the last few years. They have been demonstrated to work well even for highly nonlinear, complex models. We discuss variants of the Ensemble Kalman Inversion (EKI) aiming to improve the accuracy of the estimate by adaptively choosing the particles in the ensemble.

## [03030] Ensemble-based gradient inference for particle methods in optimization and sampling

**Format :** Talk at Waseda University

**Author(s) :** Philipp Wacker (University of Canterbury) Claudia Schillings (FU Berlin) Claudia Totzeck (University of Wuppertal)

**Abstract :** We discuss how some ensemble-based methods for optimization and sampling can be augmented by inexact estimates of the gradient of a potential function, approximated in a straightforward way from pointwise evaluation of the potential in the ensemble. This approximated gradient can be inserted in place of an exact gradient in the context of sampling methods derived from Langevin dynamics, and it can be used as an additional term in global optimization methods like Consensus-based optimization

## [05138] Less interaction with forward models in Langevin dynamics: Enrichment and Homotopy

**Format :** Talk at Waseda University

**Author(s) :** Robert Gruhlke (FU Berlin)Martin Eigel (WIAS Berlin)David Sommer (WIAS Berlin)

**Abstract :** Ensemble methods like EKS and ALDI are widely used for Bayesian inference problems but suffer from a large number of forward calls and possible lack of convergence for multimodal distributions. We propose adaptive ensemble enrichment strategies to reduce the total number of forward calls. The method is extended for more complex distributions using adapted Langevin dynamics based on a homotopy formalism. Numerical investigations on benchmark problems demonstrate the method's advantages over state-of-the-art Langevin samplers.

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00837 (2/3) : 4D @E709 [Chair: Robert Gruhlke]

## [04703] Metropolis-adjusted interacting particle sampling

**Format :** Talk at Waseda University

**Author(s) :** Bjoern Sprungk (TU Bergakademie Freiberg)Simon Weissmann (University of Mannheim)Jakob Zech (Universität Heidelberg)

**Abstract :** In recent years, various interacting particle samplers have been developed to sample from complex target distributions, such as those found in Bayesian inverse problems. These samplers are motivated by the mean-field limit perspective and implemented as ensembles of particles that move in the product state space according to coupled stochastic differential equations. The ensemble approximation and numerical time stepping used to simulate these systems can introduce bias and affect the invariance of the particle system with respect to the target distribution. To correct for this, we investigate the use of a Metropolization step, similar to the Metropolis-adjusted Langevin algorithm. We examine both ensemble- and particle-wise Metropolization and prove basic convergence of the resulting ensemble Markov chain to the target distribution. Our results demonstrate the benefits of this correction in numerical examples for popular interacting particle samplers such as ALDI, CBS, and stochastic SVGD.

## [05149] Computing log-densities of time-reversed diffusion processes through Hamilton-Jacobi-Bellman equations

**Format :** Talk at Waseda University

**Author(s) :** David Sommer Robert Gruhlke (FU Berlin)Martin Eigel (WIAS Berlin)

**Abstract :** Sampling from densities is a common challenge in uncertainty quantification. Langevin dynamics are a popular tool for this task but rely on certain properties of the log-density. To assimilate a larger class of distributions, a time-inhomogeneous drift term can be defined using intermediate log-densities. We propose learning these log-densities by propagation of the target distribution through an Ornstein-Uhlenbeck process, solving the associated Hamilton-Jacobi-Bellman equation using an implicit scheme and compressed polynomials for spatial discretization.

## [04723] Simulation of Wasserstein gradient flows with low-rank tensor methods for sampling

**Format :** Talk at Waseda University

**Author(s) :** Vitalii Aksenov (Weierstrass Institute for Applied Analysis and Stochastics)Martin Eigel (Weierstrass Institute for Applied Analysis and Stochastics)

**Abstract :** We try to adapt the Eulerian methods for Wasserstein gradient flows for high-dimensional problems such as Bayesian inversion, importance sampling and generative modelling by utilizing low-rank tensor methods. The normalized density is approximated in tractable format, which allows additional application to density estimation and rare event detection. An ODE governing the evolution of samples can be defined with help of intermediate density and flux variables, linking the approach to particle methods.

## [05014] Overparameterization of Deep ResNet: Zero Loss and Mean-Field Analysis

**Format :** Talk at Waseda University

**Author(s) :** Zhiyan Ding (University of California, Berkeley)Qin Li (University of Wisconsin, Madison)Shi Chen (University of Wisconsin, Madison)Stephen Wright (University of Wisconsin, Madison)

**Abstract :** In this talk, I will mainly focus on using mean-field analysis to analyze the overparameterization of neural networks. Finding parameters in a deep neural network (NN) that fit training data is a nonconvex optimization problem, but a basic first-order optimization method (gradient descent) finds a global optimizer with the perfect fit (zero-loss) in many practical situations. In this talk, I will investigate this phenomenon in the case of Residual Neural Networks (ResNet) with smooth activation functions in a limiting regime in which both the number of layers (depth) and the number of weights in each layer (width) go to infinity. First, I will rigorously show that the gradient descent for parameter training becomes a gradient flow for a probability distribution that is characterized by a partial differential equation (PDE) in the large-NN limit. Next, I will introduce the conditions that make sure the solution to the PDE converges in the training time to a zero-loss solution. Together, these results suggest that the training of the ResNet gives a near-zero loss if the ResNet is large enough.

00837 (3/3) : 4E @E709 [Chair: Philipp Wacker]

## [04766] Wasserstein Steepest Descent Flows for Discrepancy Flows with Riesz Kernels

**Format :** Talk at Waseda University

**Author(s) :** Johannes Hertrich (TU Berlin)Robert Beinert (TU Berlin)Gabriele Steidl (TU Berlin)

**Abstract :** We introduce Wasserstein steepest descent flows based on the geometric Wasserstein tangent space. These are locally absolutely continuous curves in the Wasserstein space whose tangent vectors point into a steepest descent direction of a given functional. This allows the use of Euler forward schemes instead of minimizing movement schemes introduced by Jordan, Kinderlehrer and Otto. Under certain assumptions, we show that there exists a unique Wasserstein steepest descent flow which coincides with the Wasserstein gradient flow. For the special example of interaction energies with non-smooth Riesz kernels, we derive analytic formulas for the corresponding Wasserstein steepest descent flows.

## [04729] Neural Wasserstein Gradient Flows for Discrepancies with Riesz Kernels

**Format :** Talk at Waseda University

**Author(s) :** Fabian Altekrüger (HU Berlin/ TU Berlin)Johannes Hertrich (TU Berlin)Gabriele Steidl (TU Berlin)

**Abstract :** Wasserstein gradient flows of maximum mean discrepancy (MMD) functionals with non-smooth Riesz kernels show a rich structure as singular measures can become absolutely continuous ones and conversely. We propose to approximate the backward scheme of Jordan, Kinderlehrer and Otto for computing such Wasserstein gradient flows as well as a forward scheme for so-called Wasserstein steepest descent flows by neural networks (NNs). Since we cannot restrict ourselves to absolutely continuous measures, we have to deal with transport plans and velocity plans instead of usual transport maps and velocity fields. Indeed, we approximate the disintegration of both plans by generative

NNs which are learned with respect to appropriate loss functions. For the interaction energy we provide analytic formulas for Wasserstein schemes starting at a Dirac measure. Finally, we illustrate our neural MMD flows by numerical examples.

## [00838] Perspectives in Artificial Intelligence and Machine Learning in Materials Chemistry, 2nd edition

**Session Time & Room :**

00838 (1/2) : 3C (Aug.23, 13:20-15:00) @D102

00838 (2/2) : 3D (Aug.23, 15:30-17:10) @D102

**Type :** Proposal of Minisymposium

**Abstract :** Artificial Intelligence has led to a paradigm shift in investigation in Materials Chemistry, with Machine Learning allowing informatics-based systematic calculations, predictions and discovery based on material databases pushing beyond the intrinsic limitations of first-principles calculations. The successful application requires development of novel methodologies inspired by the frontends of materials development in close synergy between Mathematics and Information Technology, areas where interdisciplinary collaborations are crucial and yet to date in their early phases.

**Organizer(s) :** CESANA Pierluigi, NGUYEN DINH Hoa, PACKWOOD Daniel, STAYKOV Aleksandar

**Classification :** 62P35, 68T05, 68Q32

**Minisymposium Program :**

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00838 (1/2) : 3C @D102 [Chair: STAYKOV Aleksandar]

## [01431] Discovery of New Materials by Quantum Calculations and Artificial Intelligence

**Format :** Talk at Waseda University

**Author(s) :** David Samuel Rivera Rocabado (Hiroshima University)Mika Aizawa (Hiroshima University)Takayoshi Ishimoto (Hiroshima University)

**Abstract :** Integrating artificial intelligence into real system first-principles calculations has the potential to transform the field of materials science and, ultimately, the world in which we live. In this presentation, the modeling and the prediction of the CO adsorption/activation on Ru nanoparticles exemplify that our new approach can be universally applied to predict the catalytic properties of any existing material and be used for the discovery of more functionalized materials.

## [05452] Causal analysis of materials functionality by combining topological data analysis and physical model

**Format :** Talk at Waseda University

**Author(s) :** Masato Kotsugi (Tokyo University of Science)

**Abstract :** Microscopic image data is key to developing low-power, high-speed electronic devices. However, the complex interactions in nanoscale magnetic materials are difficult to understand. We developed a new functional design theory called “extended Landau free energy model” that combines persistent homology and machine learning with free energy to automate the interpretation of the microscopic image. This model illustrates the physical mechanism and critical location of magnetization reversal and proposes a device structure with low energy consumption.

## [05575] Machine learning for materials chemistry and chemical biology

**Format :** Talk at Waseda University

**Author(s) :** Daniel Packwood (Kyoto University)

**Abstract :** This talk will review three recent success stories involving machine learning in materials science and chemistry: (1) the simulation of on-surface molecular self-assembly processes using machine-learned potentials and a novel genetic algorithm; (2) the design of a new organic semiconducting material with targeted band gap by a combination of unsupervised and supervised learning; (3) the prediction and verification of a new chemical compound for inducing cardiac tissue differentiation of stem cells.

## [01449] Topological descriptor of thermal conductivity in amorphous Si

**Format :** Online Talk on Zoom

**Author(s) :** Emi Minamitani (Osaka University)Takuma Shiga (AIST)Makoto Kashiwagi (Aoyama Gakuin University)Ippei Obayashi (Okayama University)

**Abstract :** In this talk, we analyze the relationship between the atomic configuration of amorphous Si and the thermal conductivity of the material. A topological descriptor constructed by persistent homology successfully predicts the thermal conductivity using machine learning, and from the machine learning model, we can extract medium-range order structures related to thermal conductivity using inverse analysis of persistent homology. <http://doi.org/10.1063/5.0093441>

## [05561] Fully automatized optimization of ring-opening reactions in lactone derivatives via 2-step machine learning

**Format :** Talk at Waseda University

**Author(s) :** Aleksandar Staykov (Kyushu University) Pierluigi Cesana (kyushu university)

**Abstract :** Cyclization and cycloreversion of organic compounds are fundamental kinetic processes in the design of functional molecules, molecular machines, and nano-switches. We present a fully automatic computational platform for the design of a class of 5- and 6- membered ring lactones by optimizing the ring-opening reaction rate. Starting from a minimal initial parent set, our program generates iteratively cascades of pools of candidate lactone derivatives where optimization and down-selection are performed not requiring human supervision at any stage. We use Density Functional Theory combined with transition state theory to elucidate the exact mechanism leading to the lactone ring opening. Based on the analysis of the reaction pathway and the frontier molecular orbitals, we identify a simple descriptor that can easily correlate with the reaction rate. The program is successful in identifying a large class of lactone derivatives with enhanced ring-opening properties. Our platform is modular and our current implementation for lactone could be further generalized to more complex systems via substitution of the quantum chemical and fingerprinting modules.

## [01724] A Trial for the Realization of Material Pattern Informatics Using Interpretable AI

**Format :** Talk at Waseda University

**Author(s) :** Yoh-ichi Mototake (Hitotsubashi University)

**Abstract :** It has been recently reported that highly accurate classification, regression, and generation can be achieved by interpolative modeling of complex scientific data using machine learning models with high expressive power, such as deep neural networks (DNNs). However, many of the machine learning models used there are nonlinear functions with a large number of parameters, making the interpretation of the training results very difficult. In thermodynamics, Gibbs extended the theory of thermodynamics, which was the theory of heat engines, to chemical reactions, which was a great development in science. This shows that science has been greatly advanced by the scientific insight of human beings, who derive general principles beyond mere interpolation models and boldly extrapolate them. On the other hand, it is sometimes difficult to apply such insights to systems with complex non-periodic structures, such as those found in nonlinear and nonequilibrium phenomena. To address this situation, we believe that it is important to collaborate between machine learning, which is good at building interpolation models for complex data, and humans, who can make bold extrapolations based on scientific insights, and are developing methods for interpreting machine learning training results to bridge the gap between the two.

In this presentation, we will discuss our recent research on machine learning frameworks that collaborate with scientists trying to reveal complex pattern dynamics in materials and their applications.

## [01688] Toward Functional Polymer Informatics

**Format :** Talk at Waseda University

**Author(s) :** Koichiro Kato (Kyushu University)

**Abstract :** Although materials informatics has made remarkable progress in recent years, its application to functional polymers remains unexplored. Reasons for this include the lack of established methods for incorporating the higher-order structure of functional polymers as a feature in machine learning and the lack of data. In this talk, I will present our recent results on building models for predicting properties from published data and extracting features of functional polymers using coarse-grained simulation.

## [01335] Understanding the role of defects and disorder in polycrystalline materials

**Format :** Talk at Waseda University

**Author(s) :** Kulbir K Ghuman (Institut national de la recherche scientifique)

**Abstract :** The functionality of the materials used for energy applications is critically determined by the physical properties of small active regions such as dopants, dislocations, interfaces, grain boundaries, etc. The capability to manipulate and utilize the inevitable disorder in materials, whether due to the finite-dimensional defects (such as vacancies, dopants, grain boundaries) or due to the complete atomic randomness (as in amorphous materials), can bring innovation in designing energy materials. With the increase in computational material science capabilities, it is now possible to understand the complexity present in materials due to various defects resulting in pathways

required for optimizing their efficiencies. In this talk, I will provide a critical overview of such computational advancements specifically for designing realistic materials with various types of defects. I will discuss the traditional approaches (implemented via tools such as density functional theory, and molecular dynamics) as well as modern approaches such as machine learning that exist for understanding the impact of defects and disorder present in polycrystalline materials, thereby identifying future opportunities for energy materials design and discovery.

## [00840] Efficient and scalable solvers and algorithms for multiscale phenomena

### **Session Time & Room :**

00840 (1/3) : 1D (Aug.21, 15:30-17:10) @E802

00840 (2/3) : 1E (Aug.21, 17:40-19:20) @E802

00840 (3/3) : 2C (Aug.22, 13:20-15:00) @E802

**Type :** Proposal of Minisymposium

**Abstract :** Many physical systems involve interactions between different scales in space and/or time, which usually stem from the coexistence of complex micro-structures and phenomena taking place at much larger scales.

Prominent examples of multiscale systems are biological tissues, composed of millions of cells but treated as a continuum, with scale separations in both space and time.

The focus of this minisymposium is on efficient and scalable numerical methods, solvers and high performance software, which can solve such complex systems on modern HPC computing architectures.

**Organizer(s) :** Nicolas A. Barnafi, Ngoc Mai Monica Huynh, Luca F. Pavarino

**Classification :** 65Nxx, 65Mxx, 65Fxx

**Minisymposium Program :**

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00840 (1/3) : 1D @E802 [Chair: Luca Pavarino]

## [02988] A multiscale preconditioner for simulating blood flows in artery with aneurysm

**Format :** Talk at Waseda University

**Author(s) :** Xiao-Chuan Cai (University of Macau)

**Abstract :** In this talk, we discuss some recent development of numerical methods for the simulation of blood flows in patient-specific arteries with aneurysm. Depending on the branching geometry and the patient parameters, the flow can be quite complicated with local vortex structures, but the principal component of the flow is always along the centerline of the artery. Based on this observation, we introduce a two-scale domain decomposition method for unsteady incompressible Navier-Stokes equations in three-dimensional complex patient-specific arteries, and the key component of the preconditioner is a parameterized one-dimensional unsteady Navier-Stokes or Stokes coarse problem defined along the centerline of the artery. The one-dimensional preconditioner and some overlapping three-dimensional subdomain preconditioners are combined additively to form the two-scale method via interpolations using radial basis functions. The most important feature of the method is that the cost of solving the coarse problem is nearly neglectable compared with the subdomain solver. Numerical experiments indicate that the proposed method is highly effective and robust for complex arteries with many branches and aneurysm. This is a joint work with Yingzhi Liu and Fenfen Qi.

## [04469] Spectral Element discretizations in cardiac electrophysiology: a matrix-free approach

**Format :** Talk at Waseda University

**Author(s) :** Pasquale Claudio Africa (mathLab, SISSA International School for Advanced Studies, Trieste)Matteo Salvador (Stanford University)Paola Gervasio (Università degli Studi di Brescia)

**Abstract :** We propose a high-order Spectral Element Method (SEM) matrix-free solver for the numerical solution of cardiac electrophysiology. We compare it to SEM with Numerical Integration and demonstrate that increasing the local polynomial degree leads to improved accuracy and faster computations than reducing the mesh size. Our matrix-free approach, enhanced by a suitable implementation of a Geometric Multigrid (GMG) preconditioner,

yields up to 45(\times) speed-up compared to a conventional matrix-based solver. Several numerical experiments are analyzed.

## [03783] Monolithic solution strategies for large-scale computational problems from physiology and astrophysics

**Format :** Online Talk on Zoom

**Author(s) :** pietro benedusi (Simula Research Laboratory )Rolf Krause (Università della Svizzera italiana)Patrick Zulian (Università della Svizzera italiana)

**Abstract :** Currently, many problems in applied mathematics result in large-scale computational challenges which require the use of massively parallel machines and scalable solution strategies to minimize the time to solution. In this talk, we present monolithic strategies to numerically solve partial differential equations, for various applications. These strategies consist in framing, whenever possible, a computational problem in a large and possibly sparse (non) linear system which can be solved, in parallel, combining efficient preconditioning techniques and Krylov methods. By contrast, many traditional staggered approaches are based on the solution of a sequence of smaller computational problems. An example of such a paradigm can be found when solving evolutionary problems, where a monolithic strategy (also known as all-at-once approach) can be used, resulting in the assembly of large a space-time system with a block Toeplitz structure, in contrast to standard sequential time-stepping techniques. In this context, we consider the space-time discretization of the anisotropic diffusion equation, using isogeometric analysis in space and a discontinuous Galerkin approximation in time. Drawing inspiration from a former spectral analysis of space-time operators, we propose a parallel multigrid preconditioned GMRES method. The application of this multilevel space-time strategy to non-linear reaction-diffusion problems from electrophysiology (i.e. the monodomain equation and the EMI model) will be also discussed, considering comparison with other recently developed methods. Moreover, we present a monolithic approach to simulate radiative transfer in stellar atmospheres; in this scenario, we present a matrix-free implementation of a multi-fidelity preconditioner. Through simulations on massively parallel systems, we show how monolithic strategies can improve software scalability and discuss the trade-offs of this approach.

## [04869] Platform Portable Distributed Solvers and Preconditioners in Cardiac Simulations

**Format :** Talk at Waseda University

**Author(s) :** Fritz Goebel (Karlsruhe Institute of Technology)Hartwig Anzt (Karlsruhe Institute of Technology)Terry Cojean (Karlsruhe Institute of technology)Marcel Koch (Karlsruhe Institute of Technology)

**Abstract :** In the European MICROCARD project we work on simulating the electrophysiology of the human heart with a new Cell-by-Cell model. The model's high resolution and the resulting linear systems pose a computational challenge. In this talk we report on recent developments on scaleable Krylov Methods and Preconditioners in the open source library Ginkgo that we aim to leverage in these simulations.

00840 (2/3) : 1E @E802 [Chair: Luca Pavarino]

## [03815] Overlapping Schwarz methods for Isogeometric analysis based on generalized B-splines

**Format :** Talk at Waseda University

**Author(s) :** Durkbin Cho (Dongguk University)

**Abstract :** Isogeometric analysis (IGA) is an innovative numerical methodology for the solution of partial differential equations (PDEs), introduced by Hughes, that potentially allows for a direct connection with CAD, thus providing a much easier and exact representation of the computational domain in a wide range of applications. Generalized B-splines (GB-splines) are a special class of Tchebycheff B-splines that are smooth piecewise function with sections in more general spaces. GB-splines allow for an exact representation of conic sections as well as transcendental curves and thus they become very attractive for geometrical modeling and numerical simulation. They have been proposed as an attractive tool in isogeometric analysis. Since then, isogeometric analysis based on GB-splines have been studied. In this talk, we present overlapping Schwarz preconditioners for {\sf elliptic} and {\sf biharmonic} problems discretized with isogeometric analysis based on GB-splines. An h-analysis of the proposed preconditioners shows an optimal convergence rate bound. Numerical results in two- and three-dimensional tests confirm our theory and also illustrate the good convergence properties of the preconditioner with respect to the discretization parameters.

## [03711] Higher Order Time Integration for EMI Cardiac Electrophysiology Simulations with Nested Subset Selection and BDDC Preconditioning

**Format :** Talk at Waseda University

**Author(s) :** Fatemeh Chegini (Zuse Institute Berlin(ZIB))Martin Weiser (Zuse Institute Berlin(ZIB))

**Abstract :** Cardiac electrophysiology simulations call for adaptive methods due to locality of solution features. Traditional mesh refinement and coarsening approaches incur significant overheads. We investigate a novel approach using nested subset selection for algebraic degrees of freedom in hierarchical spectral deferred correction methods. This enables multi-rate integration with minimal overhead, and reduces the computational cost significantly. We also propose a novel domain decomposition preconditioner of BDDC type for cell-by-cell electrophysiology models and show numerical results.

## [03593] Adaptive BDDC preconditioners for 3D divergence free virtual element discretizations of the Stokes equations.

**Format :** Talk at Waseda University

**Author(s) :** Tommaso Bevilacqua (University of Milan)Franco Dassi (University of Milano-Bicocca)Stefano Zampini (King Abdullah University of Science and Technology,)Simone Scacchi (University of Milan)

**Abstract :** The balancing domain decomposition by constraints (BDDC) preconditioners are domain decomposition methods based on the subdivision of the computational domain of a partial differential equation (PDE) into non-overlapping subdomains.

We apply BDDC to solve PDEs discretized by Virtual Element Methods (VEM) proving scalability and quasi-optimality of the algorithm. Numerical results with adaptively generated coarse spaces confirm the method's robustness in the presence of large jumps in the viscosity and with high-order VEM discretizations.

## [03487] Efficient solvers for models of personalized whole heart electromechanics

**Format :** Talk at Waseda University

**Author(s) :** Matthias Gsell (Medical University of Graz)Christop Augustin (Medical University of Graz)Karli Gillette (Medical University of Graz)Alexander Jung (Medical University of Graz)Gernot Plank (Medical University of Graz)

**Abstract :** Anatomically accurate computer models of four-chamber electromechanics, which are able to replicate electromechanical function of an individual patient's heart show high potential for both clinical and industrial applications such as diagnostics, treatment optimization and device development. Methodology used to obtain a first fully mechanistic whole-heart electromechanics models with non-invasively personalized electrophysiology and calibrated mechanical and vascular function will be presented. We demonstrate goodness of fit of the calibrated model, and validation against common physiological principles.

00840 (3/3) : 2C @E802 [Chair: Nicolas A. Barnafi]

## [02611] An efficient parallel interpolation algorithm with applications to multi-physics simulation of cardiac radiofrequency ablation

**Format :** Talk at Waseda University

**Author(s) :** Massimiliano Leoni (Johann Radon Institute for Computational and Applied Mathematics)Argyrios Petras (RICAM-Johann Radon Institute for Computational and Applied Mathematics)Luca Gerardo-Giorda (JKU and RICAM)

**Abstract :** In this talk we discuss modelling and simulation of Cardiac Radiofrequency Ablation, a clinical procedure used to treat some forms of cardiac arrhythmia by accessing the patient's heart with a catheter and burning it locally to make it electrically insulating.

By its nature, this problem requires a complex multi-physics approach, which in turn yields many computational challenges.

In particular, we will focus on parallel interpolation, a trivial-looking step that is crucial to a performant implementation

## [04831] A nonlinear preconditioning strategy for solving phase-field fracture problems in a constrained minimization framework

**Format :** Talk at Waseda University

**Author(s) :** Hardik Kothari (Università della Svizzera Italiana)Alena Kopaničáková (Brown University)Rolf Krause (Università della Svizzera Italiana)

**Abstract :** The phase-field approach to fracture allows one to model crack propagation, branching, and merging. Despite its robust modeling properties, solving this problem is computationally challenging due to the non-convex, non-smooth, highly nonlinear, and ill-conditioned nature of the underlying energy function. We propose a field-split-based additive/multiplicative Schwarz preconditioned Newton method to solve the fracture problem by employing a right preconditioner that can handle inequality constraints. The robustness of the method will be shown using numerical examples.

## [04801] Multi-scale modelling and simulation: EMI models, 3D-1D transport, and DG methods

**Format :** Talk at Waseda University

**Author(s) :** Rami Masri (Simula Research Laboratory)Marius Zeinhofer (Simula Research Laboratory)Miroslav Kuchta (Simula Research Laboratory)Marie Rognes (Simula Research Laboratory )

**Abstract :** In this presentation, we discuss several of our findings on a variety of multi-scale models and their discretizations. First for the EMI equations which are used to model excitable tissue, we formulate and analyse discontinuous Galerkin interior penalty formulations. The practical advantages of such an approach are that (i) it can be implemented in any finite element library without additional multimesh/mixed-dimensional features, and that (ii) black box multigrid solvers perform well. Second, we formulate coupled time dependent 3D-1D models of transport used to model a variety of phenomena. The modeling and the discretisation errors for finite element approximations are discussed.

## [04846] SCALABLE SOLVERS FOR BULK-SURFACE MATERIALS UNDERGOING SPINODAL DECOMPOSITION

**Format :** Talk at Waseda University

**Author(s) :** stefano zampini (KAUST)Luis Espanh (University of Nottingham)Luca Heltai (SISSA)Hector Gomez (Purdue University)

**Abstract :** In this work, we present numerical results for two- and three-dimensional bulk-surface materials undergoing spinodal decomposition. The emphasis will be on the numerical implementation using the deal.II framework, and on the solution of the nonlinear equations using the PETSc library.

## [00843] Innovative numerical methods for complex PDEs

**Session Time & Room :**

00843 (1/2) : 4D (Aug.24, 15:30-17:10) @E702

00843 (2/2) : 4E (Aug.24, 17:40-19:20) @E702

**Type :** Proposal of Minisymposium

**Abstract :** Many problems in science and engineering involve multi-physical processes where their complex interactions occur at a wide range of spatial and temporal scales. They can be modeled by a set of nonlinear PDEs, each representing different physical phenomena. Numerical solutions of such problems remain a quite challenging task due to the presence of multiple spatial and time scales. The goals of this minisymposium are first to present some of latest developments in numerical methods for such complex PDEs, and second to bring together experts, young researchers, and students working in this field to exchange ideas and to initiate collaborations.

**Organizer(s)** : Vu Thai Luan, Amanda Diegel, Aaron Rapp

**Classification** : 65M22, 65M60, 65M06, 65L04

**Minisymposium Program :**

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00843 (1/2) : 4D @E702 [Chair: Vu Thai Luan]

## [01855] Accelerating nonlinear solvers with continuous data assimilation

**Format** : Talk at Waseda University

**Author(s)** : Leo Rebholz (Clemson University)

**Abstract** : We show how continuous data assimilation can be used to accelerate convergence in nonlinear solvers for steady PDE. We prove that for incompressible flow problems, with sufficient measurement data the linear convergence rate of Picard iterations can be improved. Numerical tests illustrate the theory.

## [01739] Unconditionally stable numerical methods for Cahn-Hilliard-Navier-Stokes-Darcy system with different densities and viscosities

**Format** : Online Talk on Zoom

**Author(s)** : Xiaoming He (Missouri University of Science and Technology)Yali Gao (Northwestern Polytechnical University)Daozhi Han (University at Buffalo)Ulrich Rüde (Friedrich-Alexander-University of Erlangen-Nuremberg)

**Abstract** : In this presentation, we consider the numerical modeling and simulation via the phase field approach for coupled two-phase free flow and two-phase porous media flow of different densities and viscosities. The model consists of the Cahn-Hilliard-Navier-Stokes equations in the free flow region and the Cahn-Hilliard-Darcy equations in porous media that are coupled by several domain interface conditions. It is showed that the coupled model satisfies an energy law. Then we first propose a coupled unconditionally stable finite element method for solving this model and analyze the energy stability for this method. Furthermore, based on the ideas of pressure stabilization and artificial compressibility, we propose an unconditionally stable time stepping method that decouples the computation of the phase field variable, the velocity and pressure of free flow, the velocity and pressure of porous media, hence significantly reduces the computational cost. The energy stability of this decoupled scheme with the finite element spatial discretization is rigorously established. We verify numerically that our schemes are convergent and energy-law preserving. Numerical experiments are also performed to illustrate the features of two-phase flows in the coupled free flow and porous media setting.

## [01884] Modified exponential Rosenbrock methods to increase their accuracy

**Format** : Online Talk on Zoom

**Author(s)** : Begoña Cano (Universidad de Valladolid)María Jesús Moreta (Universidad Complutense de Madrid)

**Abstract** : In this talk a technique will be described to avoid order reduction when integrating nonlinear initial boundary value

problems with exponential Rosenbrock methods. The technique does not require to impose any stiff order conditions

but to add some terms related to the information on the boundary. Theoretical results on local and global error will be

given as well as some numerical comparisons.

## [01971] Low Regularity Integrators for Semilinear Parabolic Equations with Maximum Bound Principles

**Format** : Talk at Waseda University

**Author(s)** : Cao-Kha Doan (Auburn University)Lili Ju (University of South Carolina)Thi-Thao-Phuong Hoang (Auburn University)Katharina Schratz (Sorbonne Université)

**Abstract** : This work is concerned with structure-preserving, low regularity time integration methods for a class of semilinear parabolic equations of Allen-Cahn type. Important properties of such equations include maximum bound principle (MBP) and energy dissipation law; for the former, that means the absolute value of the solution is pointwisely bounded for all the time by some constant imposed by appropriate initial and boundary conditions. The model equation is first discretized in space by the central finite difference, then by iteratively using Duhamel's formula, first and second-order low regularity integrators (LRIs) are constructed for time discretization of the semi-discrete system. The proposed LRI schemes are proved to preserve the MBP and the energy stability in the discrete sense. Furthermore, some semi-discrete and fully-discrete error estimates are also successfully derived under the part\_2

low regularity requirement that the corresponding exact solution is only assumed to be continuous in time. Numerical results show that the proposed LRI schemes can be more accurate and achieve better convergence than classic exponential time differencing (ETD) schemes, especially when the interfacial parameter approaches zero.

00843 (2/2) : 4E @E702 [Chair: Amanda Diegel]

## [02261] A tourist's guide to operator splitting

**Format :** Talk at Waseda University

**Author(s) :** Raymond Spiteri (University of Saskatchewan) Siqi Wei (University of Saskatchewan)

**Abstract :** Operator splitting is the dirty little thing we all do when a differential equation is too hard to solve monolithically. Many questions abound, however, regarding how to split a given problem, and many observations and "common knowledge" lack a theoretical understanding. In this talk, I take you on a tour through some of the practical aspects of operator splitting and while touching on some of the folklore that exists around it.

## [02294] Adaptive exponential Runge--Kutta methods for stiff PDEs

**Format :** Talk at Waseda University

**Author(s) :** Luan Vu Thai (Mississippi State University)

**Abstract :** Exponential Runge-Kutta methods have shown to be well-suited for stiff parabolic PDEs. Their constructions require solving stiff order conditions which involve matrix functions. Current schemes allow using with constant stepsizes only. In this talk, we will derive new schemes of high order which not only fulfill the stiff order conditions in the strong sense and but also support variable step sizes implementation. Numerical experiments are given to illustrate accuracy and efficiency of the new schemes.

## [02660] The Dual-Wind Discontinuous Galerkin Method for Hamilton-Jacobi Equations

**Format :** Talk at Waseda University

**Author(s) :** Aaron Rapp (University of the Virgin Islands)

**Abstract :** A discontinuous Galerkin (DG) finite-element interior calculus is used as a common framework to describe various DG approximation methods for second-order elliptic problems. This framework allows for the approximation of both primal and variational forms of second order differential equations. In this presentation, we will study the error from using the dual-wind DG derivatives to approximate the the solution to stationary and time-dependent Hamilton-Jacobi equations. Some analytical results will be presented, along with numerical examples that verify these results.

# [00851] Mathematics for Big Data and Artificial Intelligence: models and challenges

**Session Time & Room :** 4C (Aug.24, 13:20-15:00) @E504

**Type :** Proposal of Minisymposium

**Abstract :** The availability of huge amounts of data and the application of AI techniques are considered as the fourth industrial revolution, but extracting meaningful knowledge and transparent decisions from the data is not a trivial task.

Mathematics is the 'language' on which are based the existing algorithms for data processing and for AI. This minisymposium is organized within the ECMI SIG "Mathematics for Big Data and AI". The talks in this minisymposium will present and discuss how Mathematics can play a leading role in improving the reliability, computational efficiency, and transparency of the existing techniques for big data analysis and AI.

**Organizer(s) :** Alessandra Micheletti, Natasa Krejic

**Classification :** 62Pxx, 62R40, 68T07, 65K10, 68Txx

**Minisymposium Program :**

00851 (1/1) : 4C @E504 [Chair: Alessandra Micheletti]

## [01685] Equivariant non-expansive operators as a bridge between TDA and geometric deep learning

**Format :** Talk at Waseda University

**Author(s) :** Patrizio Frosini (University of Bologna)

**Abstract :** Group equivariant non-expansive operators (GENEOs) have been recently introduced as mathematical tools for approximating data observers when data are represented by real-valued or vector-valued functions (<https://rdcu.be/bP6HV>). The use of these operators is based on the assumption that data interpretation depends on the observers' geometric properties. In this talk we will illustrate some recent results, showing how GENEOs can make available an interesting link between topological data analysis and geometric deep learning.

## [01623] a new machine learning paradigm for protein pocket detection based on Group Equivariant Non Expansive Operators

**Format :** Talk at Waseda University

**Author(s) :** Alessandra Micheletti (Università degli Studi di Milano)Giovanni Bocchi (Università degli Studi di Milano)Patrizio Frosini (Università degli Studi di Bologna)Carmine Talarico (Dompè Farmaceutici)Filippo Lunghini (Dompè Farmaceutici)Andrea Beccari (Dompè Farmaceutici)Carmen Gratteri (University Magna Grecia Catanzaro)Alessandro Pedretti (Università degli Studi di Milano)

**Abstract :** Protein pockets detection is a key problem in the context of drug development, since the ability to identify a small number of potential binding sites, allows to speed up drug discovery procedures. In this talk we will show how Group Equivariant Non Expansive Operators (GENEOs) can be used to build a geometrical machine learning method, able to detect protein pockets better than ML techniques already in use, but being based only on 17 unknown parameters.

## [01528] SLiSeS: Subsampled Line Search Spectral Gradient Method for Finite Sums

**Format :** Online Talk on Zoom

**Author(s) :** Stefania Bellavia (University of Florence)Natasa Krejic (University of Novi Sad)Natasa Krklec Jerinkic (University of Novi Sad)Marcos Alejandro Raydan (NOVA University Lisbon)

**Abstract :** In this paper, we aim to exploit advantages of spectral method in stochastic optimization framework, especially in mini-batch subsampling case which is often used in Big Data setup. In order to let the spectral coefficient explore the spectrum of the approximate Hessian, we keep the same sample for several iterations before we subsample again. We analyze conditions for almost sure convergence and present initial numerical results that show the advantages of the proposed method.

## [01698] Interpretable models for large-scale tabular datasets

**Format :** Online Talk on Zoom

**Author(s) :** Claudia Soares (NOVA School of Science and Technology)

**Abstract :**

The purpose of this work is two-fold: on the one hand, to demonstrate that machine learning models can be considered a powerful alternative to predicting real-world variables in high-stakes scenarios, and, on the other hand, to propose a new method that is empirically the state-of-the-art rule-based method for large datasets. We accompany our method with tailored algorithms for fast learning in large datasets.

## [00854] Control and stabilization of PDEs: recent advances and applications

**Session Time & Room :**

00854 (1/3) : 2C (Aug.22, 13:20-15:00) @G605

00854 (2/3) : 2D (Aug.22, 15:30-17:10) @G605

00854 (3/3) : 2E (Aug.22, 17:40-19:20) @G605

**Type :** Proposal of Minisymposium

**Abstract :** As control problems arise naturally from engineering and physics, control theory has attracted a lot of attention in the last century. In recent decades, the study of control problems from PDEs' point of view has developed quickly, finding natural connections with fluid mechanics, microlocal analysis, stochastic analysis, and many applications such as traffic flow regulations, lane manufacturing, crowd motion, and biology, etc. We focus on these new developments, which cover a wide range of problems from observability to quantitative stabilization and finite-time stabilization across many different types of systems from subelliptic equations to conservation laws to hybrid systems.

**Organizer(s) :** Shengquan Xiang, Maria Teresa Chiri, Amaury Hayat, Qi Lü

**Classification :** 35L04, 76B15, 49J20, 93D15, 93C95

**Minisymposium Program :**

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00854 (1/3) : 2C @G605 [Chair: Amaury Hayat]

## [02524] Quantitative rapid stabilization of some PDE models

**Format :** Talk at Waseda University

**Author(s) :** Shengquan Xiang (Peking University)

**Abstract :** Quantitative stabilization is an active research topic in PDEs' control theory, namely to construct explicit feedback laws as a control to make the closed-loop system stable together with quantitative estimates. In this presentation, we will talk about some recent progress in this topic including the Frequency Lyapunov method for the stabilization of Navier-Stokes equations and the Fredholm backstepping method for the stabilization of water waves.

## [02863] Generalized Fredholm-backstepping transformation

**Format :** Talk at Waseda University

**Author(s) :** Ludovick Gagnon (Inria Nancy)Christophe Zhang (Inria Nancy)Amaury Hayat (Ecole des Ponts Paristech)Shengquan Xiang (Peking University)Swann Marx (CNRS)

**Abstract :** The backstepping method for PDEs, introduced over 20 years ago, is a powerful method to prove the rapid stabilisation of linear PDEs. The Fredholm alternative, introduced by Coron and Lü, quickly proved to provide a systematic approach to the backstepping method based on the spectral behaviour of the PDE as well as controllability assumptions. We present in this talk recent advances on sufficient conditions for the Fredholm-backstepping method in an abstract setting.

## [02944] Indirect controllability of linear constant coefficients parabolic-transport systems

**Format :** Talk at Waseda University

**Author(s) :** Pierre Lissy (Université Paris-Dauphine)

**Abstract :** I will present controllability properties of mixed systems of linear parabolic-transport equations, with possibly nondiagonalizable diffusion matrix, on the 1D torus, coupled by constant coupling terms. The distributed control acts through a constant matrix, with possibly less controls than equations. In small time or for not regular enough initial data, these systems are never controllable, whereas in large time, null-controllability holds, for regular initial data, iff a spectral Kalman rank condition is verified.

## [03571] Optimal Control of Moving Sets

**Format :** Talk at Waseda University

**Author(s) :** Maria Teresa Chiri (Queen's University)

**Abstract :** We consider a controlled reaction-diffusion equation, modeling the spreading of an invasive population. Our goal is to derive a simpler model, describing the controlled evolution of a contaminated set. We first analyze the optimal control of 1-dimensional traveling wave profiles. Using Stokes' formula, explicit solutions are obtained, which in some cases require measure-valued optimal controls. Then we introduce a family of optimization problems for a moving set and show how these can be derived from the original parabolic problems, by taking a sharp interface limit. Assuming that the initial contaminated set is convex, we prove that an eradication strategy is optimal if and only if at each given time the control is active along the portion of the boundary where the curvature is maximal. We then consider the eradication problem with geographical constraints, and derive necessary and sufficient conditions for the existence of a solution.

00854 (2/3) : 2D @G605 [Chair: Maria Teresa Chiri]

## [04439] On the boundary controllability of conservation laws with boundary and source controls

**Format :** Talk at Waseda University

**Author(s) :** Fabio Ancona (University of Padova)Khai Tien Nguyen (North Carolina State University)

**Abstract :** We will discuss local and global controllability results for hyperbolic conservation laws on a bounded domain, where the control acts through a time dependent source term in combination with the boundary controls. We shall investigate first this problem for scalar conservation laws with a not necessarily convex flux. Next, we shall address the problem of extending these results to the case of rich systems of conservation laws.

## [02947] Advances on structural controllability of ensembles

**Format :** Talk at Waseda University

**Author(s) :** Bahman Gharesifard (UCLA)

**Abstract :** Ensemble control studies the problem of steering the state of a large population of systems, or a continuum, using a finite number of controllers. The problem has historic ties to control of partial differential equations, with many applications including quantum ensembles in spectroscopy, control of large limits of complex networks with few inputs, and recently in the study of universal approximation of neural networks. The purpose of this talk is to study a suit of structural controllability results for linear ensemble systems, where the objective is to identify structural properties that generically render the state of the ensemble — or some statistical properties of the profile over the parametrization space, for instance the average or higher moments — controllable. The latter provides a necessary and critical complement to full structural ensemble controllability which is hard to achieve in multiparameter settings. For the case where the statistical property of interest is the average, we provide a graph-theoretic characterization of structural controllability. Along the way of establishing this result, we hint at a conjecture on minimal “complexity” controllers and relate it a conjecture on invertibility of a sparse version of Hilbert matrices, which is open for most parts.

## [03282] Second microlocalization and optimal decay for the Bouendi-Grushin damped wave equation

**Format :** Talk at Waseda University

**Author(s) :** Chenmin Sun (CNRS(Université Paris Est Créteil))Victor Arnaiz (Nantes Université)

**Abstract :** The Bouendi-Grushin damped-wave operator is a hypoelliptic operator with a distributional damping. This presentation introduces the second microlocalization method for obtaining the optimal resolvent estimate for the operator under varying damping conditions.

## [04573] Controls on Networks: Modeling, Learning and Applications

**Format :** Talk at Waseda University

**Author(s) :** Yue Wang (Friedrich-Alexander-Universität Erlangen-Nürnberg)

**Abstract :** This talk is an introduction of controllability properties and methods for networked 1D hyperbolic systems based on results obtained by the speaker and her collaborators in recent years. Modelling, analysis of the underlying dynamics and exact controllability of several physical models will be presented at first. Some recent numerical experiments with Physics-Informed Neural Networks (PINNs) show interesting possibilities for future research on the interface between control and machine learning.

00854 (3/3) : 2E @G605 [Chair: Shengquan Xiang]

## [03018] Stabilization of 1D evolution systems: new approaches

**Format :** Talk at Waseda University

**Author(s) :** Amaury Hayat (Ecole des Ponts ParisTech)

**Abstract :** We discuss recent advances in the F-equivalence (or Fredholm backstepping) method. This consists in reformulating the stabilization problem and to find a control operator such that the PDE system can be inversely mapped to a simpler PDE system. Surprisingly powerful, this approach offers the possibility to treat very general classes of systems. We will also examine traffic flow stabilization. Finally, we will briefly discuss some results on AI for mathematics.

## [02943] Feedback stabilization and inverse problem for a nonlocal transport equation

**Format :** Talk at Waseda University

**Author(s) :** Zhiqiang Wang (Fudan University)

**Abstract :** In this talk, we will show some results on feedback stabilization and inverse problems for a transport equation with nonlocal velocity. This model arises in the control of semiconductor manufacturing systems which have a highly re-entrant character. Firstly we obtain a semi-global stabilization result by using a time-varying feedback control. Secondly with the help of certain feedback control, we recover the velocity function from the measurements.

## [04252] The controllability of a special class of coupled wave systems

**Format :** Talk at Waseda University

**Author(s) :** Jingrui Niu (Sorbonne Université)Pierre Lissy (Université Paris-Dauphine)

**Abstract :** I will present an exact controllability result for coupled wave systems with two distinct speeds. A distributed scalar control function is effective in a subdomain satisfying the geometric control conditions and acts on only one speed. We establish compatibility conditions, which are associated with the particular coupling structure. Furthermore, the exact controllability holds in these compatible spaces if and only if the coupling structure satisfies an operator Kalman rank condition.

## [02522] Geometry of observable sets

**Format :** Talk at Waseda University

**Author(s) :** gengsheng wang (Tianjin University)

**Abstract :** We introduce several observability inequalities in some abstract setting. Then for some concrete evolution equations, such as the heat equation and the Schrodinger equations on the whole space, we give the characterizations of the observable sets such that the aforementioned inequalities hold. We further give some comments.

# [00866] BEM and related methods for advanced applications

**Session Time & Room :** 5D (Aug.25, 15:30-17:10) @E704

**Type :** Proposal of Minisymposium

**Abstract :** Since its early days, the Boundary Element Method (BEM) has been selected as an accurate, scalable and reliable tool in computational science and engineering. In particular, in the last three decades, the number of its applications to cutting edge academic/industrial fields has impressively grown up. This Minisymposium is devoted to application aspects of BEM and its main goal is to bring together experts in this field, belonging to different international research groups, to discuss on the most recent advances and current open challenges on fast and innovative strategies for real-life applications.

**Organizer(s) :** Luca Desiderio, Alessandra Aimi, Chiara Guardasoni

**Classification :** 65N38

**Minisymposium Program :**

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00866 (1/1) : 5D @E704 [Chair: Luca Desiderio]

## [04974] Time domain boundary elements and mesh refinements

**Format :** Online Talk on Zoom

**Author(s) :** Heiko Gimperlein (University of Innsbruck)

**Abstract :** We discuss recent and on-going progress for time-domain boundary element methods for wave and elastodynamic problems, with a focus on locally refined meshes. Solutions of the time-dependent equations exhibit singularities due to geometry (corners), mixed or nonlinear (contact) boundary conditions. We discuss well-posed formulations for such problems as well as their approximation on locally refined meshes by h- and hp-versions. A priori and a posteriori estimates for the approximation error are presented for both the weakly singular and the hypersingular integral

part\_2

equations. The a posteriori estimates lead to an adaptive mesh refinement procedure. Numerical experiments illustrate the theoretical results. (joint with A. Aimi, G. Di Credico, C. Oezdemir and E. P. Stephan)

## [05091] On improving the flexibility of an IgA-BEM multi-patch code

**Format :** Online Talk on Zoom

**Author(s) :** Alessandra Sestini (Università di Firenze)

**Abstract :** Two flexibility improvements are introduced of a 3D multi-patch IgA-BEM approach for Helmholtz based on B-spline tailored numerical integration. The first concerns the possibility of developing the discretization in non-conforming  $C^0$  multi-patch spline spaces, thus ensuring adaptivity at the patch level. The second consists in the capability of using non uniform tensor product formulations of the adopted quadrature rules which are based on quasi-interpolation. This allows us to deal with non-smooth inter-patch junctions.

## [04013] Solving 2D linear elastic wave equations by scalar potentials

**Format :** Online Talk on Zoom

**Author(s) :** Silvia Falletta (Polytechnic University of Turin)

**Abstract :** This talk focuses on the simulation of 2D soft scattering elastic wave propagation in isotropic homogeneous media, using the scalar potential decomposition in the time-harmonic regime. For problems defined in bounded domains, a Virtual Element Method (VEM) with varying mesh sizes and degrees of accuracy is proposed to approximate the two scalar potentials. For unbounded domains, a boundary element method is coupled with the VEM.

## [04853] Time-Domain BEM for the resolution of Elastodynamic Contact Problems

**Format :** Online Talk on Zoom

**Author(s) :** Giulia Di Credico (University of Parma) Alessandra Aimi (University of Parma) Heiko Gimperlein (University of Innsbruck)

**Abstract :** We investigate a boundary element method (BEM) for the dynamic contact between a linearly elastic body and a rigid obstacle. The so-called Signorini problem is formulated on the boundary as a variational inequality for the elastodynamic equations, for which we consider a mixed formulation solvable by time-domain BEM coupled with Uzawa algorithm. Both theoretical and algorithmic aspects are discussed and numerical experiments, presented for different 2D geometries, show the optimal performance of the proposed approach.

# [00869] Theory, numerics and data driven methods for fluids

**Session Time & Room :**

00869 (1/3) : 5B (Aug.25, 10:40-12:20) @D403

00869 (2/3) : 5C (Aug.25, 13:20-15:00) @D403

00869 (3/3) : 5D (Aug.25, 15:30-17:10) @D403

**Type :** Proposal of Minisymposium

**Abstract :** Despite recent progress in the study of turbulent fluids, to date our mathematical understanding of it remains fundamentally incomplete. Furthermore, recent work on non-uniqueness of weak solutions and lack of global well-posedness of fluid equations, make their study even more pertinent and urgent. This mini-symposium will bring together researchers at all career stages to share their recent results on the interplay of topics such as uniqueness, regularity, boundary-layer theory, asymptotic dynamics and their connections to data assimilation, parameter estimation, machine and physics-informed deep learning algorithms, porous media flow simulations, and the study of statistical and stochastic solutions.

**Organizer(s) :** Animikh Biswas, Jing Tian

**Classification :** 76R50, 65P40

**Minisymposium Program :**

## [01423] Parameter analysis in continuous data assimilation for three-dimensional Brinkman-Forchheimer-extended Darcy model

**Format :** Online Talk on Zoom

**Author(s) :** Débora Aparecida Francisco Albanez (Universidade Tecnológica Federal do Paraná)

**Abstract :** Analytical results of the long-time behavior of three-dimensional Brinkman-Forchheimer-extended Darcy model in the context that the parameters related to the damping nonlinear term are unknown is presented. We show estimates in  $L^2$  and  $H^1$  for large-time error between the true solution and the assimilated solution, which is constructed with the unknown damping parameters and observational measurements obtained continuously in time from a continuous data assimilation technique.

## [04819] Boundary layers for a viscous fluid in a corner domain

**Format :** Online Talk on Zoom

**Author(s) :** Anna Mazzucato (Penn State University)

**Abstract :** We study boundary layers for incompressible slightly viscous fluids in a rectangular domain when steady shears are applied to the top and bottom side. We establish the vanishing viscosity limit using various types of correctors. In particular, we introduce suitable corner layer correctors at the corners. This is joint work with Gung-Min Gie (U. Louisville) and James Kelliher (UC Riverside).

## [03465] Numerical schemes for various stochastic models in hydrodynamic

**Format :** Online Talk on Zoom

**Author(s) :** Hakima Bessaih (Florida International University)

**Abstract :** We will introduce space-time numerical schemes for some stochastic models in hydrodynamic. The models include, the stochastic Navier-Stokes equations, the Boussinesq equations and some other models in porous media. We will also discuss various rates of convergences in probability and in mean square.

## [01351] Coupling of free flow and flow in porous media

**Format :** Talk at Waseda University

**Author(s) :** Xiaoming Wang (Missouri University of Science and Technology and Southern University of Science and Technology)

**Abstract :** We present some recent progress in the study of coupled free flow and porous media flow. In particular, we show that the several competing interface boundary conditions are asymptotically equivalent at the physically importance small Darcy number regime. We also offer a coarse-grained theory in predicting the deep vs shallow convections in the case when heat convection is involved. Effective numerical algorithms will be presented if time permits.

00869 (2/3) : 5C @D403 [Chair: Vincent R Martinez]

## [01798] Wellposedness of stochastic PDEs arising in fluid dynamics

**Format :** Online Talk on Zoom

**Author(s) :** Krutika Tawri (University of California Berkeley)

**Abstract :** Stochastic forcing terms are commonly added to the governing equations to account for numerical and physical uncertainties in applications. In this talk, we will discuss recent results and new techniques in the analysis of stochastic models, arising in fluid dynamics.

## [03526] Error estimates for deep learning methods in fluid dynamics

**Format :** Talk at Waseda University

**Author(s) :** Jing Tian (Towson university) Animikh Biswas (University of Maryland, Baltimore County) Suleyman Ulusoy (American University of Ras Al Khaimah)

**Abstract :** In this talk, we provide error estimates and stability analysis of deep learning techniques for certain partial differential equations including the incompressible Navier-Stokes equations. In particular, we obtain explicit error estimates for the solution computed by optimizing a loss function in a Deep Neural Network approximation of the solution, with a fixed complexity.

## [01243] Reconstructing external driving forces in incompressible flow via low-mode observation

**Format :** Talk at Waseda University

**Author(s) :** Vincent R Martinez (CUNY Hunter College & Graduate Center)

**Abstract :** In this talk, we describe a "spectral filtering" algorithm that reconstructs an apriori unknown external force in the 2D Navier-Stokes equations. This approach was developed by Celik, Olson, and Titi (2019) in order to recover the unobserved high-mode motion of the flow provided that sufficiently many low-modes are observed and that the external force is known. It is shown how this idea can be used to simultaneously recover both the unobserved motion and unknown forcing.

## [04541] Analysis of a rotationally constrained convection model

**Format :** Talk at Waseda University

**Author(s) :** Yanqiu Guo (Florida International University)

**Abstract :** This talk is about the analysis of an asymptotically reduced system for rotationally constrained convection. This reduced system was derived from the 3D Boussinesq equations using the asymptotic theory. On the one hand, the nonlinear convection term has a reduced complexity since it contains only the horizontal gradient. On the other hand, the regularizing viscosity acts in the horizontal direction only. I will present some of our results motivated by the global regularity problem.

00869 (3/3) : 5D @D403 [Chair: Jing Tian]

## [04953] Estimation of parameters on the fly via nudging methods

**Format :** Talk at Waseda University

**Author(s) :** Jared P Whitehead (Brigham Young University)

**Abstract :** We demonstrate the utility of an algorithm that allows for the estimation and recovery of parameters in a dissipative dynamical system. Rigorous justification of the algorithm is established for specific settings, and numerical simulations are used to demonstrate that it works in various settings and for different circumstances including the estimation of a full forcing function and additive and multiplicative parameters.

## [04093] Uniform Boundedness of Entropy to Compressible Navier-Stokes Equations with Vacuum

**Format :** Talk at Waseda University

**Author(s) :** Jinkai Li (South China Normal University)

**Abstract :** In the presence of vacuum, the physical entropy for polytropic gases behave singularly and it is thus hard to study its dynamics. In this talk, we present some recent studies on the uniform boundedness of the entropy to the viscous compressible ideal gas in the presence of vacuum either at the far field or on the gas-vacuum interface. It will be shown in this talk that, in the case that the vacuum presents at the far fields only, the uniform boundedness of the entropy can be propagated locally or globally if the initial density decays slowly, while if the initial density decays sufficiently fast, the entropy becomes unbounded immediately after the initial time, in particular, the entropy tends to infinity at the far field.

## [05089] A unified framework for the analysis of accuracy and stability of a class of data assimilation methods for the Navier-Stokes equations

**Format :** Talk at Waseda University

**Author(s) :** Michal Branicki (University of Edinburgh)Animikh Biswas (University of Maryland Baltimore County)

**Abstract :** Bayesian state estimation of a dynamical system utilising a stream of noisy measurements is important in many geophysical and engineering applications, where nonlinearities, high (or infinite) dimensionality of the state space, and sparse observations pose key challenges for deriving efficient and accurate data assimilation techniques. We develop a unified framework for the analysis of several well-known and empirically efficient data assimilation techniques derived from various Gaussian approximations of the Bayesian filtering problem for geophysical-type dissipative dynamics with quadratic nonlinearities. Our approach also elucidates the links between the approximate-Bayesian and control-theoretic approaches to data assimilation. We consider the 'model' dynamics governed by the two-dimensional incompressible Navier-Stokes equations and observations given by noisy measurements of finite volume elements, modal or nodal points of the velocity field. In this setup the

continuous-time data assimilation techniques, the so-called 3DVar and EnKF (Ensemble Kalman filter), are given by stochastically forced Navier–Stokes equations. We derive rigorous conditions for the (time-asymptotic) accuracy and stability of these algorithms and show the relevance of the so-called covariance inflation and localisation for assuring the necessary bounds. These conditions involve an interplay between the resolution of the observations associated with the covariance operator underlying the data assimilation algorithms and, for the first time, elucidate the properties of the EnKF as well as of the 3DVar for a general covariance operator which is common and relevant for volume and nodal observations.

## [00874] Recent advances in the analysis and numerics for phase-field models

**Session Time & Room :** 2E (Aug.22, 17:40-19:20) @G606

**Type :** Proposal of Minisymposium

**Abstract :** Phase-field models are a powerful tool for studying the dynamics of phase transformations and internal structures in materials. In recent years, there have been significant advances in the analysis and numerical techniques for phase-field models. These advances range from innovative solution concepts and modelling approaches to structure inheriting numerical schemes together with adaptive mesh refinements.

These methods have led to a deeper understanding of the underlying physics and have had a wide range of applications in areas such as materials science, biology, and engineering.

**Organizer(s) :** Dietmar Hömberg, Robert Lasarzik

**Classification :** 35Q99, 65M12

**Minisymposium Program :**

00874 (1/1) : 2E @G606 [Chair: Robert Lasarzik]

## [02784] Existence of weak solutions to an anisotropic electrokinetic flow model

**Format :** Talk at Waseda University

**Author(s) :** Luisa Plato (WIAS)Robert Lasarzik (Weierstrass Institut of Applied Analysis and Stochastics Berlin )Dietmar Hömberg (Weierstrass Institut of Applied Analysis and Stochastics Berlin )

**Abstract :** In this talk the existence proof of weak solutions in three space dimensions to an anisotropic Navier—Stokes—Nernst—Planck—Poisson system is presented.

This models the electrokinetic flow induced by charged particles dissolved in a liquid crystals with constant director field. The existence proof relies on an approximating scheme and weak sequential compactness of the approximating sequence, which follows from the energy law. Weak—strong uniqueness is proven via the relative energy inequality.

## [02502] Global existence for a singular nonlocal phase field system with inertial term

**Format :** Talk at Waseda University

**Author(s) :** Shunsuke Kurima (Tokyo University of Science)

**Abstract :** This talk deals with a nonlocal phase field system with inertial term. Colli-Colturato (2018) have established existence of solutions to a phase field system related to the entropy balance. Also, Colli-Grasselli-Ito (2002) have proved existence for a parabolic-hyperbolic Penrose-Fife phase field system. However, singular nonlocal phase field systems with inertial term seem to be not studied yet.

The present work asserts that we can derive existence for a singular nonlocal phase field system with inertial term.

## [02824] A structure-preserving scheme for the Liu-Wu model

**Format :** Talk at Waseda University

**Author(s) :** Makoto Okumura (Konan University)

**Abstract :** Recently, the Cahn-Hilliard equation with new dynamical boundary conditions has been proposed by Liu and Wu. This model has characteristic conservation laws in that each mass of the interior of the domain and the boundary are conserved. In addition, the total energy dissipation law holds. In this talk, we propose a structure-

preserving scheme for the Liu-Wu model that retains the conservation and dissipation laws in a discrete sense and show the mathematical and numerical results.

## [02783] Analysis of an Allen--Cahn system in two scale topology optimization

**Format :** Talk at Waseda University

**Author(s) :** Robert Lasarzik (Weierstrass Institut of Applied Analysis and Stochastics Berlin )Dietmar Höemberg (Weierstrass Institut of Applied Analysis and Stochastics Berlin )Moritz Ebeling-RumpIn this talk, we consider an Allen—Cahn system with the obstacle potential that guarantees mass conservation. This equation is coupled to two linear elasticity equations and a nonlocal operator. This system emerged from an algorithm for a (Weierstrass Institut of Applied Analysis and Stochastics Berlin )

**Abstract :** In this talk, we consider an Allen—Cahn system with the obstacle potential that guarantees mass conservation. This equation is coupled to two linear elasticity equations and a nonlocal operator. This system emerged from an algorithm for a problem in two-scale topology optimization using the phase-field approach. We prove the existence of weak solutions for the associated inclusion and comment on different connections of the solvability concept and the numerical algorithm.

## [00876] Inverse Problems in Partial Differential Equations and Graphs

**Session Time & Room :**

00876 (1/2) : 1C (Aug.21, 13:20-15:00) @G809

00876 (2/2) : 1D (Aug.21, 15:30-17:10) @G809

**Type :** Proposal of Minisymposium

**Abstract :** The minisymposium discusses recent development on inverse problems for partial differential equations on manifolds and inverse problems on graphs. Inverse problems typically study the reconstruction of system parameters and geometric or combinatorial structures from indirect measurements. They naturally appear in various imaging problems such as in geophysics, medical imaging, network tomography, material science and non-destructive testing. Many inverse problems are highly sensitive to noise, and understanding this unstable nature is important to applications. Inverse problems on manifolds and graphs in general exhibit different nature, and this minisymposium seeks new connections between them.

**Organizer(s) :** Matti Lassas, Jinpeng Lu, Lauri Oksanen

**Classification :** 35R30, 81U40, 05C50, 05C81

**Minisymposium Program :**

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00876 (1/2) : 1C @G809

## [04431] Geophysics and algebraic geometry

**Format :** Talk at Waseda University

**Author(s) :** Joonas Ilmavirta (University of Jyväskylä)

**Abstract :** Many areas of interest within the Earth are anisotropic, meaning that the speed of sound is different in different directions. It turns out that pressure waves are far better behaved than shear waves, but fortunately the different polarizations are coupled together through algebraic geometry. I will explain the surprising power of algebraic geometry in the study of anisotropic inverse problems.

## [03655] Retrieving coupled Yang-Mills-Higgs fields

**Format :** Talk at Waseda University

**Author(s) :** Xi Chen (Fudan University)Matti Lassas (University of Helsinki)Gabriel Paternain (University of Cambridge)Lauri Oksanen (University of Helsinki)

**Abstract :** The pure Yang-Mills theory is only able to describe the behavior of massless gauge bosons. But experiments show massive gauge bosons do exist. According to the Higgs mechanism of mass generation, the mass of gauge bosons is acquired through the interactions with Higgs bosons. Therefore, the combined Yang-Mills-Higgs

Lagrangian together with its Euler-Lagrange equation is of great scientific significance. We show that one can detect the coupled Yang-Mills-Higgs fields from active local measurements of Yang-Mills-Higgs equations.

### [03095] Inverse problems for the graph Laplacian

**Format :** Talk at Waseda University

**Author(s) :** Jinpeng Lu (University of Helsinki)

**Abstract :** We study the discrete version of Gel'fand's inverse spectral problem, of determining the graph structure of a finite weighted graph from the spectral data of its graph Laplacian. We prove that the problem is uniquely solvable under a novel Two-Points Condition. We also consider an inverse problem for random walks on finite graphs and its unique solvability under this condition. This is a joint work with E. Blästen, H. Isozaki and M. Lassas.

### [03169] Quantum computing algorithms for inverse problems on graphs

**Format :** Talk at Waseda University

**Author(s) :** Joonas Ilmavirta (University of Jyväskylä) Matti Lassas (University of Helsinki) Jinpeng Lu (University of Helsinki) Lauri Oksanen (University of Helsinki) Lauri Ylinen (University of Helsinki)

**Abstract :** We consider a quantum algorithm for an inverse travel time problem on a graph. This problem is a discrete version of the inverse travel time problem encountered in seismic and medical imaging and the boundary rigidity problem studied in Riemannian geometry. We also consider the computational complexity of the inverse problem, and show that the quantum algorithm has a quadratic improvement in computational cost when compared to the standard classical algorithm.

00876 (2/2) : 1D @G809

### [05146] Density results in the Calderon problem

**Format :** Online Talk on Zoom

**Author(s) :** Mikko Salo (University of Jyväskylä)

**Abstract :** We will discuss recent density results for products of harmonic functions, and applications of these results to inverse problems such as the linearized Calderon problem and the Calderon problem for nonlinear partial differential equations. The emphasis will be on the geometric setting that corresponds to anisotropic conductivity coefficients given by a Riemannian metric.

### [03644] Rellich type theorem for lattice Hamiltonians

**Format :** Talk at Waseda University

**Author(s) :** Hiroshi Isozaki (University of Tsukuba)

**Abstract :**

We announce results for a Rellich type theorem on a locally perturbed periodic lattice containing square, triangular and hexagonal lattices.

This is a joint work with K. Ando and H. Morioka.

### [04868] Continuum limits of discrete Schrödinger operators on lattices

**Format :** Talk at Waseda University

**Author(s) :** Yukihide Tadano (Tokyo University of Science)

**Abstract :** We consider continuum limit problems of discrete Schrödinger operators defined on lattices.

We show that the corresponding Schrödinger operators on the Euclidean space are obtained as the above continuum limits in the generalized norm resolvent sense.

This talk is based on joint work with Shu Nakamura.

# [00877] Mathematical and Computational Methods for Topological Materials

## **Session Time & Room :**

00877 (1/2) : 5B (Aug.25, 10:40-12:20) @D405

00877 (2/2) : 5C (Aug.25, 13:20-15:00) @D405

## **Type :** Proposal of Minisymposium

**Abstract :** Topological materials are a class of quantum materials whose properties are preserved under topological transformations. The delicate structures of these materials admit novel and subtle propagating wave patterns which are immune to backscattering from disorder and defects. Recent years have witnessed vast of new experiments and theories about the wave phenomena in topological materials. The goal of this minisymposium is to bring together theoretical and applied researchers in these areas to discuss recent advances in the mathematical theories and physical applications. Topics will include analysis of the underlying governing equations, numerical methods on computing edge states, and experimental realizations.

**Organizer(s) :** Hailong Guo, Emmanuel Lorin, Xu Yang

**Classification :** 78M10, 78A48, 47A70, 35P99

## **Minisymposium Program :**

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00877 (1/2) : 5B @D405 [Chair: Emmanuel Lorin]

## [03694] Computation of phononic crystals using the PG finite element method

### **Format :** Talk at Waseda University

**Author(s) :** Liqun Wang (China University of Petroleum-Beijing)

**Abstract :** Phononic crystals are composite materials with periodic distribution of two or more media. The difficulty of computing the band structure of the phononic crystals lies in capturing the complex geometry and jump conditions effectively on the interface between the scatterer and the matrix. This talk will present the Petrov-Galerkin Finite Element Method for the band structure computation of phononic crystals, and the properties of various materials are also discussed.

## [05337] Conically degenerate spectral points of the periodic Schrödinger operator

### **Format :** Talk at Waseda University

**Author(s) :** Yi Zhu (Tsinghua University)

**Abstract :** Conical spectral points on the dispersion bands are the origin of many novel topological phenomena, including various topological phases. I will first review recent mathematical theories on these points, especially Fefferman & Weinstein's results (JAMS 2012) on 2D Dirac points, which paved the way for rigorous justifications of such points. Then I will focus on our recent progress in constructing 3-fold Weyl points at which two energy bands intersect conically with an extra band sandwiched in between. We give the existence of such points in the spectrum of the 3-dimensional Schrödinger operator  $H = -\Delta + V(x)$  with  $V(x)$  being in a large class of periodic potentials. This is the first rigorous result on the existence of 3-fold Weyl points for a broad family of 3D continuous Schrödinger equations. Our result extends Fefferman-Weinstein's pioneering work to higher dimensions and multiplicities.

## [02726] Frozen Gaussian sampling for wave equations

### **Format :** Talk at Waseda University

**Author(s) :** Lihui Chai (Sun Yat-sen University)Ye Feng (Sun Yat-sen University)Zhennan Zhou (Peking University)

**Abstract :** We introduce the frozen Gaussian sampling (FGS) algorithm to solve the wave equation in the high-frequency regime. The FGS algorithm is a Monte Carlo sampling strategy based on the frozen Gaussian approximation, which greatly reduces the computation workload in wave propagation and reconstruction. We propose feasible and detailed procedures to implement the FGS algorithm, and we analyze the error caused by the sampling algorithm with Gaussian initial conditions and WKB initial conditions respectively.

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00877 (2/2) : 5C @D405

## [05595] Unfitted Computation of edge modes in photonic graphene

**Author(s)** : Hailong Guo (The University of Melbourne )Yi Zhu (Tsinghua University)Xu Yang (University of California Santa Barbara)

**Abstract** : Photonic graphene, a photonic crystal with honeycomb structures, has been intensively studied in both theoretical and applied fields. In this paper, we propose a new unfitted Nitsche's method of computing edge modes in photonic graphene with some defect. The unique feather of the methods is that they can arbitrary handle high contrast with geometric unfitted meshes. We establish the optimal convergence of methods.

## [00879] Stochastic analysis in mathematical finance

**Session Time & Room** : 4E (Aug.24, 17:40-19:20) @F412

**Type** : Proposal of Minisymposium

**Abstract** : In this minisymposium the recent advances in mathematical finance will be discussed. The topics include stochastic analysis of jump processes, stochastic optimization, partial differential equations, stochastic calculus of variations, and mathematical aspects of data science for pricing and hedging of financial products. This minisymposium will bring together researchers with the aim to stimulate discussions for both theoretical and practical advancement.

**Organizer(s)** : Takuji Arai, Tomoyuki Ichiba  
**Sponsor** : This session is sponsored by the SIAM Activity Group on Financial Mathematics and Engineering.

**Classification** : 60H30, 91G15, 91G80

**Minisymposium Program** :

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00879 (1/1) : 4E @F412 [Chair: Tomoyuki Ichiba]

## [03804] Constrained optimal stopping under a regime-switching model

**Format** : Talk at Waseda University

**Author(s)** : Takuji Arai (Keio University)

**Abstract** : We investigate an optimal stopping problem for the expected value of a discounted payoff on a regime-switching geometric Brownian motion under two constraints on the possible stopping times: only at exogenous random times and only during a specific regime. The main objectives are to show that an optimal stopping time exists as a threshold type and to derive expressions of the value functions and the optimal threshold. To this end, we solve the corresponding variational inequality and show that its solution coincides with the value functions. Some numerical results are also introduced. Furthermore, we investigate some asymptotic behaviors.

## [04565] Remarks on pathwise Itô calculus in infinite dimensions

**Format** : Talk at Waseda University

**Author(s)** : Yuki Hirai (National Institute of Technology, Tsuruoka College)

**Abstract** : The Itô–Föllmer calculus, pioneered by Föllmer (1981), is a deterministic counterpart to classical Itô's stochastic calculus. It has recently been receiving increasing attention from the viewpoint of its financial applications. In this talk, we extend some results in the Itô–Föllmer calculus to infinite dimensional settings.

## [03809] Systemic Risk and Overconfidence under Stochastic Environment

**Format** : Talk at Waseda University

**Author(s)** : Li-Hsien Sun (National Central University)

**Abstract** : We propose an optimal portfolio problem based on the mean variance criterion based on the relative performance with the feature of overconfidence. Namely, investors intend to maximize the distance between the average and minimize their own variance as well. In the meantime, they also consider the better return than the real one due to overconfidence. We illustrate systemic risk by applying the probability of the large number of defaults. Finally, the influence of overconfidence is discussed through numerical analysis.

part\_2

## [03808] Smoothness of Directed Chain Stochastic Differential Equations and Its Applications

**Format :** Talk at Waseda University

**Author(s) :** Tomoyuki Ichiba (University of California Santa Barbara )

**Abstract :** On a filtered probability space for the space of continuous functions, we shall consider a system of stochastic equations called directed chain stochastic differential equations for a pair of stochastic processes whose marginal distributions in the path space are identical and their joint distribution is uniquely determined by the system of equations with the distributional constraints. In this talk we discuss the smoothness of the solutions of the equations under some regular conditions and introduce its applications of such systems to the stochastic filtering problem and to the generative adversarial network problem in finance.

## [00882] Geometric Shape Generation II: Design

**Session Time & Room :**

00882 (1/3) : 5B (Aug.25, 10:40-12:20) @F403

00882 (2/3) : 5C (Aug.25, 13:20-15:00) @F403

00882 (3/3) : 5D (Aug.25, 15:30-17:10) @F403

**Type :** Proposal of Minisymposium

**Abstract :** This mini-symposium is based on the JSIAM activity group “Geometric Shape Generation”, and aims at exhibiting the latest research in this activity group and relevant researchers, especially putting its focus on the design. We discuss the mathematical aspects of design and analysis of shapes under various settings, and special curves and surfaces useful for generating desirable shapes on CAD.

**Organizer(s) :** Yoshiki Jikumaru, Kenji Kajiwara, Kenjiro T. Miura, Masaaki Umehara

**Classification :** 53A04, 53A05, 53A10, 53A35, 53A70

**Minisymposium Program :**

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00882 (1/3) : 5B @F403 [Chair: Masaaki Umehara]

## [01784] Construcion of discrete zero mean curvature surfaces in Euclidean and Lorentz-Minkowski spaces

**Format :** Talk at Waseda University

**Author(s) :** Masashi Yasumoto (Tokushima University)

**Abstract :** In this talk we first introduce discrete timelike minimal surfaces in Lorentz-Minkowski 3-space. Compared with other discrete zero mean surfaces, discrete timelike minimal surfaces possess richer mathematical structures. Starting from discrete timelike minimal surfaces, we construct discrete zero mean curvature surfaces in Lorentz-Minkowski 3-space that can have both spacelike and timelike parts. As an application, we construct discrete holomorphic functions and new discrete minimal surfaces in Euclidean space.

## [01406] Bifurcation of the trajectory shape in self-propelled motions

**Format :** Talk at Waseda University

**Author(s) :** Hiroyuki Kitahata (Chiba University)

**Abstract :** We consider the motion of a self-propelled particle which is driven by the surface tension gradient originating from the concentration of the chemicals released from the particle itself. First, we discuss the trajectory shape of the particle confined in a circular region. Next, we discuss the bifurcation of the motion for the motion observed in the system with a self-propelled particle and a passive particle.

## [01771] Construction of weaving structures by standard realizations with repulsive interactions

**Format :** Talk at Waseda University

**Author(s) :** Eriko Shinkawa Motoko Kotani (Tohoku University) Hisashi Naito (Nagoya University)

**Abstract :** We consider weaving structures. Let  $T$  be two sets of threads in 2-dimensional Euclidean space, where all the threads in each set are parallel and assign up/down information at their intersections. To find a suitable configuration of  $T$  in 3-dimensional Euclidean space, we take the energy that is given by the standard realization with repulsive interactions introduced by A. Dechant et al. We discuss the existence of energy minimizing configurations, which are called weaving structures.

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00882 (2/3) : 5C @F403 [Chair: Yoshiki Jikumaru]

## [01581] Generation of $\kappa$ -Space Curve

**Format :** Talk at Waseda University

**Author(s) :** DAN WANG (Shizuoka University) Tadatoshi Sekine (Shizuoka University) Shin Usuki (Shizuoka University) Kenjiro Takai Miura (Department of Mechanical Engineering, Shizuoka University)

**Abstract :** The  $\kappa$ -curve is a recently published interpolating spline which consists of quadratic Bezier segments passing through input points at the loci of local curvature extrema. But their interpolation can only deal with planar curves. Therefore, in this research We propose a method that enables to extend this representation to deal with space curves in a new scheme called  $\kappa$ -space curves

## [01561] The uniqueness theorem on the shape of free-form curves

**Format :** Talk at Waseda University

**Author(s) :** Kenjiro Takai Miura (Shizuoka University) R.U. Gobithaasan (University Malaysia Terengganu) Md Yushalify Misro (University Science Malaysia) Tadatoshi Sekine (Shizuoka University) Shin Usuki (Shizuoka University)

**Abstract :** We will discuss about the shape uniqueness theorem for curves defined by three or more control points and show several examples of applications of the theorem.

## [01775] Construction of $\kappa$ -Curve Using Fractional Bézier Curve

**Format :** Talk at Waseda University

**Author(s) :** Syed Ahmad Aidil Adha Said Mad Zain (Universiti Sains Malaysia) Md Yushalify Misro (Universiti Sains Malaysia) Kenjiro Takai Miura (Department of Mechanical Engineering, Shizuoka University)

**Abstract :** The  $\kappa$ -curve is one of the famous curves that has been applied as a curvature pen tool in Adobe Illustrator® and Photoshop®. The  $\kappa$ -curve has an excellent property where the local maxima of curvature have occurred at the control points. This will prevent the formation of cusps and loops. In this work, the construction of the  $\kappa$ -curve will be shown by using the fractional Bézier curve with the help of fractional continuity.

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00882 (3/3) : 5D @F403 [Chair: Kenjiro Takai Miura]

## [01764] Generation of Aesthetic Shape by Integrable Geometry

**Format :** Talk at Waseda University

**Author(s) :** Kenji Kajiwara (Institute of Mathematics for Industry, Kyushu University)

**Abstract :** We consider log-aesthetic curves (LAC), a family of planar curves developed in industrial design, as curves that car designers regard as “aesthetic.” We present a new mathematical framework of LAC on the theory of integrable systems and similarity geometry. Using this framework, LAC is shown to be a similarity geometry analogue of Euler’s Elastica. Based on this, we present generalizations of LAC to space curves and surfaces, which may be useful for generating aesthetic shapes.

## [01613] On the relationship between mimetic discretization and discrete exterior calculus

**Format :** Talk at Waseda University

**Author(s) :** Sampei Hirose (Shibaura Institute of Technology)

**Abstract :** The mimetic discretization is a general framework for the discretization of differential operators using differential forms, including finite element and finite volume methods. On the other hand, the discrete exterior calculus is a method for dealing with differential forms on discrete spaces and is used in computer graphics and other applications. In this talk, the relationship between the mimetic discretization and the discrete exterior calculus developed by Anil Hirani and others will be discussed.

## [01640] Quantifying the shape of data using Topological Data Analysis

**Format :** Talk at Waseda University

**Author(s) :** R U Gobithaasan (University Malaysia Terengganu)Kenjiro Takai Miura (Shizuoka University)Pawel Dlotko (Dioscuri Centre in Topological Data Analysis, Mathematical Institute, Polish Academy.)

**Abstract :** Topological Data Analysis (TDA) encodes the global structure and overall connectivity of high dimensional dataset, hence revealing the linearity, distribution, clusters and groups abnormality. TDA has two methodologies namely Persistent homology which produces Persistence Diagram and, TDA Mapper which is a graph representing the structure of the data. In this talk, we will discuss both the methodologies with numerical examples for efficient implementation.

## [01713] Biangular coordinates: moving forward

**Format :** Talk at Waseda University

**Author(s) :** Rushan Ziatdinov (Keimyung University)

**Abstract :** A bipolar coordinate system, known as biangular coordinates, uses two angles rather than one to describe the location of a point in a plane. Most common curves' equations in biangular coordinates are still unknown, and little research has been done on the features of this coordinate system and its potential uses. This work aims to advance our understanding of biangular coordinates.

## [00886] Numerical methods for stochastic partial differential equations

**Session Time & Room :**

00886 (1/2) : 1C (Aug.21, 13:20-15:00) @E506

00886 (2/2) : 1D (Aug.21, 15:30-17:10) @E506

**Type :** Proposal of Minisymposium

**Abstract :** Nowadays, the stochastic partial differential equations (SPDEs) are widely accepted as suitable models to understand complex phenomena and have been successfully applied in a broad range of areas including acoustics, electromagnetic and fluid dynamics. It is highly desirable to build efficient and reliable numerical methods, and to analyze their qualitative and quantitative properties: convergence rates (in strong and weak senses), long time behavior, approximation of invariant distributions, preservation of invariants, etc. This Minisymposium aims to provide a platform to show the significance and recent developments in numerical methods for SPDEs, and to foster interactions between academic and industrial researchers.

**Organizer(s) :** Charles-Edouard Bréhier, Jianbo Cui

**Classification :** 65C30, 60H35, 60H15

**Minisymposium Program :**

00886 (1/2) : 1C @E506 [Chair: Jianbo Cui]

## [05603] Convergence Analysis of splitting up method for nonlinear filtering problem

**Format :** Talk at Waseda University

**Author(s) :** Yanzhao Cao (Auburn University)

**Abstract :** Abstract: We consider a nonlinear filtering model where correlated Wiener processes and point processes drive observations. We first derive a Zakai equation that provides the filter solution's unnormalized probability density function. We then use a splitting-up technique to decompose the Zakai equation into three stochastic differential equations. Based on this, we construct a splitting-up approximate solution. We will present a half-order convergence result. Additionally, we will present a finite difference method to create a time semi-discrete approximate solution to the splitting-up system and prove its half-order convergence to the exact solution of the Zakai equation. Finally, we present some numerical experiments to demonstrate the theoretical analysis.

## [04327] CLT for approximating ergodic limit of SPDEs via a full discretization

**Format :** Talk at Waseda University

**Author(s) :** Chuchu Chen (Academy of Mathematics and Systems Science, Chinese Academy of Sciences) Tonghe Dang (Academy of Mathematics and Systems Science, Chinese Academy of Sciences) Jialin Hong (Academy of Mathematics and Systems Science, Chinese Academy of Sciences) Tau Zhou (Academy of Mathematics and Systems Science, Chinese Academy of Sciences)

**Abstract :** The approximation of the ergodic limit is of fundamental importance in many applications. In this talk, we focus on characterizing quantitatively the fluctuations between the ergodic limit and the time-averaging estimator of the full discretization for the parabolic stochastic partial differential equation. We establish a central limit theorem, which shows that the normalized time-averaging estimator converges to a normal distribution with the variance being the same as that of the continuous case, where the scale used for the normalization corresponds to the temporal strong convergence rate of the considered full discretization.

## [04355] Energy regularized approximations for stochastic logarithmic Schrodinger equation

**Format :** Talk at Waseda University

**Author(s) :** Jianbo Cui (Hong Kong Polytechnic University) Jialin Hong (Academy of Mathematics and Systems Science, Chinese Academy of Sciences) Liying Sun (Capital Normal University)

**Abstract :** In this talk, we first prove the global existence and uniqueness of the solution of the stochastic logarithmic Schroedinger (SlogS) equation driven by additive noise or multiplicative noise. The key ingredient lies on the regularized stochastic logarithmic Schroedinger (RSlogS) equation with regularized energy and the strong convergence analysis of the solutions of RSlogS equations. Then we present energy regularized numerical schemes and their strong convergence rates.

## [05599] Density approximation for stochastic heat equation

**Format :** Online Talk on Zoom

**Author(s) :** Derui Sheng (The Hong Kong Polytechnic University) Chuchu Chen (Academy of Mathematics and Systems Science, Chinese Academy of Sciences) Jianbo Cui (Department of Applied Mathematics, The Hong Kong Polytechnic University) Jialin Hong (Academy of Mathematics and Systems Science, Chinese Academy of Sciences)

**Abstract :** This talk presents the numerical approximation of the density of the stochastic heat equation via the accelerated exponential Euler scheme. The existence and smoothness of the density of the numerical solution are proved through Malliavin calculus. By presenting a test-function-independent weak convergence analysis, we show that the convergence orders of the density in uniform convergence topology are 1/2 and nearly 1 in the nonlinear drift case and in the affine drift case, respectively.

## [03909] Space-time Discontinuous Galerkin Methods for the $\varepsilon$ -dependent Stochastic Allen-Cahn Equation with mild noise

**Format :** Online Talk on Zoom

**Author(s) :** Dimitra Antonopoulou (University of Chester)

**Abstract :** We consider the  $\varepsilon$ -dependent stochastic Allen-Cahn equation with mild space-time noise posed on a bounded domain in  $\mathbb{R}^d$ ,  $d \geq 1$ . The noise tends to rough on the sharp interface limit. This equation is numerically approximated by a space-time discontinuous in time nonlinear Galerkin scheme for which we prove existence and uniqueness. A priori and a posteriori error analysis is applied and error estimates are established.

## [05156] Finite differences method for stochastic heat equation with singular drifts.

**Format :** Online Talk on Zoom

**Author(s) :** Ludovic Michel Goudenèg (CNRS)El Mehdi Haress (Paris-Saclay University)Alexandre Richard (Paris-Saclay University)

**Abstract :** I will present the numerical approximation of the unique solution to a stochastic heat equation in dimension 1 with distributional drifts under Besov regularity and additive space-time white noise.

The approximation is based on a tamed Euler finite-difference scheme with mollified drift.

The rate of convergence of the numerical approximation towards the unique strong solution is related to the regularity of the drift.

When the Besov regularity increases and the drift becomes a bounded measurable function, we recover the rate of convergence 1/2 in space and 1/4 in time.

Some numerical simulations of the stochastic heat equation with Dirac drift or penalization drift will be presented.

## [04362] Numerical schemes and related qualitative properties for degenerate PDEs driven by Lévy noise.

**Format :** Online Talk on Zoom

**Author(s) :** Ananta Kumar Majee (Indian Institute of Technology Delhi)Soumya Ranjan Behera (Indian Institute of Technology Delhi)

**Abstract :** In this talk, we consider an operator splitting scheme and semi-discrete finite difference scheme for fractional degenerate conservation laws driven by Lévy noise and degenerate parabolic-hyperbolic PDE with Lévy noise respectively. By using necessary a-priori bounds for approximate solutions, generated by splitting scheme, and average time continuity of regularized viscous solutions together with a variant of classical Kružkov's doubling of variables approach, we prove convergence of approximate solutions to the unique BV entropy solution of the underlying problem. Moreover, the convergence analysis is illustrated by several numerical examples. Furthermore, for compactly supported initial data, we prove that the expected value of the  $L^1$ -difference between the unique entropy solution and the approximate solutions, generated by finite difference scheme, converges at a rate of order 1/7.

## [04784] Linear implicit time-stepping schemes for SPDEs with super-linearly growing coefficients

**Format :** Online Talk on Zoom

**Author(s) :** Xiaojie Wang (Central South University)Mengchao Wang (Central South University)

**Abstract :** The present talk is on strong approximations of stochastic partial differential equations (SPDEs) with polynomially growing nonlinearity and multiplicative trace-class noise. We propose and analyze a spatio-temporal discretization of the SPDEs, by incorporating a standard finite element method in space and a linear implicit Euler-type scheme for the temporal discretization. We recover the strong convergence rates of the fully discrete scheme.

# [00888] Geometric Shape Generation I: Structures

## **Session Time & Room :**

00888 (1/3) : 4D (Aug.24, 15:30-17:10) @F411

00888 (2/3) : 4E (Aug.24, 17:40-19:20) @F411

00888 (3/3) : 5B (Aug.25, 10:40-12:20) @F411

**Type :** Proposal of Minisymposium

**Abstract :** This mini-symposium is based on the JSIAM activity group “Geometric Shape Generation”, and aims at exhibiting the latest research in this activity group and relevant researchers, especially putting its focus on the structures, mechanics and analysis. We discuss origami structures and applications, discrete surfaces and shell structures, geometric modeling of specific surfaces and vibration analysis.

**Organizer(s) :** Miyuki Koiso, Makoto Ohsaki, Jun Mitani, Kento Okuda

**Classification :** 53A05, 53A17, 53Z30, 74G65, 74H45

## **Minisymposium Program :**

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00888 (1/3) : 4D @F411 [Chair: Jun Mitani]

## **[02770] Shape modeling of umbrella surfaces**

**Format :** Talk at Waseda University

**Author(s) :** Takashi Maekawa (Waseda University)Kenji Takizawa (Waseda University)Takuya Terahara (Waseda University)

**Abstract :** We introduce a geometric modeling method of the umbrella by defining the rib curves as the intersection of two bilinear patches. Furthermore, we investigate various differential geometric properties of the umbrella surface and introduce a method to unfold it onto a plane that can be used to fabricate a wooden template for cutting canopy fabrics.

## **[04221] Geometrical and structural design of pseudo-geodesic gridshells**

**Format :** Talk at Waseda University

**Author(s) :** Romain Mesnil (Ecole des Ponts ParisTech)Olivier Baverel (Ecole des Ponts ParisTech)

**Abstract :** Gridshells are efficient structures built using a network of straight members that are deformed into doubly curved shapes. In this presentation, we propose to construct gridshells with pseudo-geodesic curves, which are characterized by the equality between torsion and geodesic torsion. We show that existence of parametrization by pseudo-geodesic network is impossible when integral of Gaussian curvature is superior to an upper bound. Structural performance and fabrication are discussed with the case-study of an architectural pavilion.

## **[02774] Preliminary research on shape searching method for curved crease origami using bending deformation**

**Format :** Talk at Waseda University

**Author(s) :** Tianhao Zhang (The University of Tokyo)Ken'ichi Kawaguchi (The University of Tokyo)

**Abstract :** Curved crease origami is focused on by the researchers and designers in the field of building structure owing to the foldability and mechanical properties. In this paper, a shape searching method is proposed based on an optimization approach. This approach can form a shape close to the target surface defined by the designers. This research aims to search the shape concerning bending deformation to explores the application of curved origami to architectural structures.

## [02924] Shape design of free-form shells with specified projected membrane forces

**Format :** Talk at Waseda University

**Author(s) :** Makoto Ohsaki (Kyoto University)Yusuke Sakai (Sony Computer Science Laboratories)Taku Nakajima (Kyoto University)Riree Takeoka (Takenaka Corporation)

**Abstract :** A shape design method is proposed for membrane free-form shells modeled as a graph surface. The distribution of membrane forces projected to the plane is specified to satisfy horizontal equilibrium as a function of shear stress. The shape is determined as a solution to the vertical equilibrium equations discretized by the finite difference method. The shape is iteratively corrected to achieve the specified projected stress distribution considering the material property.

00888 (2/3) : 4E @F411 [Chair: Makoto Ohsaki]

## [05391] Singularity of Arc- and Spiral-shaped Miura-ori as Rigid-Flat-Foldable Origami Pattern

**Format :** Talk at Waseda University

**Author(s) :** Hiroyuki Tagawa (Mukogawa Women's University)

**Abstract :** Arc- and spiral-shaped Miura-ori is rigid flat-folding Origami pattern and one variational type of Miura-ori. Geometric folding lines of the spiral-shaped Miura-ori are obtained by arraying quadrilaterals with identical internal angles in the same column. The arc-shaped Miura-ori is obtained by setting equal edge lengths of the quadrilaterals in the radial direction. This study investigates the singularity of an arc- and spiral-shaped Miura-ori among the generalized Miura-ori.

## [03876] A first-order method for large-scale eigenvalue optimization problems in topology optimization

**Format :** Talk at Waseda University

**Author(s) :** Akatsuki Nishioka (The University of Tokyo)Mitsuru Toyoda (Tokyo Metropolitan University)Mirai Tanaka (The Institute of Statistical Mathematics)Yoshihiro Kanno (The University of Tokyo)

**Abstract :** Eigenvalue optimization problems arise in many situations in topology optimization when considering robustness, vibration and buckling. As topology optimization problems are often very large-scale, the semidefinite programming approach is sometimes too computationally costly. We propose an efficient optimization algorithm based on the smoothing method for large-scale eigenvalue problems. The proposed method only uses the first-order derivative of the objective function, and thus has low computational cost per iteration. It also has convergence guarantee.

## [03320] Recent advances on tension-compression mixed shell form-finding

**Format :** Talk at Waseda University

**Author(s) :** Masaaki Miki (The University of Tokyo)

**Abstract :** In architecture, thin surface structures that can withstand gravity with no bending action are called shells. Shells have special geometries that enable them to stream gravitational force toward the ground along their forms with in-plane stresses only; the process of finding these special forms is called form-finding. Researchers have pointed out that in shell form-finding, the problem can be formulated using two surfaces: the shell itself and another surface called Airy's stress function. In 2022, a novel NURBS-based computational approach that can properly handle mixed tension-compression stress states was presented by Miki et al. (note that similar methods were first introduced in Ciang Yu-Chou). Because the solutions are represented by NURBS, the partial derivatives can be computed at any point. This enables many kind of computations. In this talk, we present what kind of computation turns possible based on the solutions obtained by the proposed method.

## [02771] Developable surfaces with curved folds

**Format :** Talk at Waseda University

**Author(s) :** Miyuki Koiso (Kyushu University)

**Abstract :** Developable surfaces are surfaces which can be unfolded into the plane preserving the length of all curves on the surface. Since developable surfaces with curved folds are constructed by bending a flat sheet, they have many applications in manufacturing objects. In this talk, we give conditions of piecewise-smooth surfaces for

being developable in terms of curvatures. We also discuss variational problems for developable surfaces, geometric characterizations of their optimal solutions, and their applications to architecture.

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00888 (3/3) : 5B @F411 [Chair: Miyuki Koiso]

## [02773] Variational principle for generating discrete surfaces with piecewise constant Gaussian curvatures

**Format :** Talk at Waseda University

**Author(s) :** Kazuki Hayashi (Kyoto University)Yoshiki Jikumaru (Kyushu University)Makoto Ohsaki (Kyoto University)Takashi Kagaya (Muroran Institute of Technology)Yohei Yokosuka (Kagoshima University)

**Abstract :** We derive a method to generate triangular meshes with piecewise constant Gaussian curvatures, in which the connection between the patches is G0 continuous. Gaussian curvature flows at interior vertices and those at the internal boundary are derived from the variational principle of the energy functional. The proposed method can generate the shape of the whole surface integrally using the derived flows.

## [02776] Geometric shape generation of hanging membranes

**Format :** Talk at Waseda University

**Author(s) :** Yoshiki Jikumaru (Toyo University)Yohei Yokosuka (Kagoshima University)

**Abstract :** In this talk, we present a differential geometric formulation of hanging membranes based on the equilibrium equations in the shell membrane theory and the variational principle.

We also propose a geometric shape generation of hanging membranes.

## [05556] Proposal for a temporary structure with a mechanism capable of curved folding

**Format :** Talk at Waseda University

**Author(s) :** Yohei Yokosuka (Kagoshima University)Miyuki Koiso (Kyushu University)Kento Okuda (National Institute of Technology, Sasebo College)Toshio Honma (Kagoshima University)Jun Mitani (University of Tsukuba)

**Abstract :** Temporary housing requires the rapid supply of numerous houses after a disaster. Therefore, it is useful to use architectural structures that utilizes curved folding, which enables the immediate development of a flat board into a three-dimensional structure.

In this presentation, a pillow type box that maximizes the inner volume is adopted for the design shape, we demonstrate numerical analysis of rigid folding and scaled models of temporary structures with a mechanism capable of curved folding.

## [05623] Topology of vibrating shapes

**Format :** Talk at Waseda University

**Author(s) :** Konrad Polthier (FU Berlin)Jakub Rondomanski (FU Berlin)Carlos Andres Palma (HU Berlin)José D. Cojal González (HU Berlin)Jürgen P. Rabe (HU Berlin)

**Abstract :** Vibrations of a parameter dependent set of physical shapes exhibit characterizing topological properties. We will discuss the topology of such vibrations based on a carefully selected metric and its holonomy.

Overall, the choice of the metric embarks beyond the classical Berry connection. Applications aim at a better understanding of the topology of vibrating crystals.

# [00891] Derivative-Free Optimization Theory, Methods, and Software

**Session Time & Room :**

00891 (1/2) : 5B (Aug.25, 10:40-12:20) @D501

00891 (2/2) : 5C (Aug.25, 13:20-15:00) @D501

**Type :** Proposal of Minisymposium

**Abstract :** Derivative-free optimization methods aim to solve optimization problems based on function values without using derivatives or other first-order information. They are motivated by problems where the first-order information is expensive or impossible to obtain. Such problems emerge frequently from industrial and engineering applications, including integrated circuit design, aircraft design, and hyperparameter tuning in artificial intelligence. This minisymposium will provide a platform for researchers and practitioners in derivative-free optimization to discuss the recent advances in theory, methods, and software in this area.

**Organizer(s) :** Serge Gratton, Zaikun Zhang

**Classification :** 90C56, 90C30, 90C26, 65K05, Derivative-Free Optimization, Numerical Optimization, Nonlinear Optimization, Nonconvex Optimization

**Minisymposium Program :**

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00891 (1/2) : 5B @D501 [Chair: Zaikun Zhang]

## [03615] Stochastic Average Model Methods

**Format :** Talk at Waseda University

**Author(s) :** Matt Menickelly (Argonne)Stefan M Wild (Lawrence Berkeley National Laboratory)

**Abstract :** We consider finite-sum minimization problems in which the summand functions are computationally expensive, making it undesirable to evaluate all summands on every iteration. We present the idea of stochastic average model methods, which sample component functions according to a probability distribution on component functions that minimizes an upper bound on the variance of the resulting stochastic model. We present promising numerical results on a corresponding extension to the derivative-free model-based trust-region solver POUNDERS.

## [01372] DFO with Transformed Objectives and a Model-based Trust-region Method

**Format :** Talk at Waseda University

**Author(s) :** Pengcheng Xie (Academy of Mathematics and Systems Science (AMSS), Chinese Academy of Sciences (CAS))

**Abstract :** Derivative-free optimization, i.e., DFO, is the optimization where the derivative information is unavailable. The least Frobenius norm updating quadratic model is an essential under-determined model for derivative-free trust-region methods. We propose DFO with transformed objectives and give a model-based method with the least Frobenius norm model. We prove the existence and necessary and sufficient condition of model optimality-preserving transformations, and analyze the model, interpolation error and convergence property. Numerical results support our model and method.

## [01341] COBYQA — A Derivative-Free Trust-Region SQP Method for Nonlinearly Constrained Optimization

**Format :** Talk at Waseda University

**Author(s) :** Tom M. Ragonneau (The Hong Kong Polytechnic University)Zaikun Zhang (The Hong Kong Polytechnic University)

**Abstract :** This talk introduces COBYQA, a derivative-free trust-region SQP method for nonlinear optimization. The method builds trust-region quadratic models using the derivative-free symmetric Broyden update. An important feature of COBYQA is that it always respects bound constraints. COBYQA is competitive with NEWUOA, BOBYQA, and LINCOA while being able to handle more general problems. Most importantly, COBYQA evidently outperforms COBYLA on all types of problems.

COBYQA is implemented in Python and is publicly available at <https://www.cobyqa.com/>.

## [03192] A General Blackbox Optimization Framework for Hyperparameter Optimization in Deep Learning

**Format :** Talk at Waseda University

**Author(s) :** Edward Hallé-Hannan (Polytechnique Montréal)Sébastien Le Digabel (Polytechnique Montréal)Charles Audet (Polytechnique Montréal)

**Abstract :** Tuning the hyperparameters of a deep model is a mixed-variable BBO problem with an unfixed structure. For instance, the number of layers (a hyperparameter) affects the number of architectural hyperparameters: meta variables are introduced to model this unfixed structure. Moreover, the hyperparameter optimization problem (HPO) may also simultaneously contain categorical, integer and continuous variables. A

mathematical framework, which is compatible with direct search methods and Bayesian optimization, is proposed to tackle and model the HPO.

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00891 (2/2) : 5C @D501 [Chair: Zaikun Zhang]

## [01570] PRIMA: Reference Implementation for Powell's methods with Modernization and Amelioration

**Format :** Talk at Waseda University

**Author(s) :** Zaikun Zhang (The Hong Kong Polytechnic University)

**Abstract :** Powell developed five widely used DFO solvers, namely COBYLA, UOBYQA, NEWUOA, BOBYQA, and LINCOA. They were coded in Fortran 77 with a unique style, which poses a significant obstacle to maintaining, exploiting, or extending them. PRIMA is a project providing the reference implementation of these solvers in modern languages. We will present the current stage of PRIMA, including the bugs we have spotted in the Fortran 77 code and the improvements we have achieved.

## [00893] Higher Order-type Optimization Methods for Machine Learning

**Session Time & Room :**

00893 (1/3) : 1E (Aug.21, 17:40-19:20) @D501

00893 (2/3) : 2C (Aug.22, 13:20-15:00) @D501

00893 (3/3) : 2D (Aug.22, 15:30-17:10) @D501

**Type :** Proposal of Minisymposium

**Abstract :** Higher order optimization mechanisms are popular and powerful tools to accelerate, robustify, and enhance the performance of first order algorithms. Albeit the high and general prevalence of first order schemes, deterministic and stochastic higher order-type methods have recently gained increasing attention and have been successfully utilized to solve challenging large-scale learning tasks, reinforcement learning problems, and other big data applications. The purpose of this minisymposium is to highlight recent advances and discuss novel techniques and strategies in the development and analysis of deterministic and stochastic higher order-type methods for large-scale minimization problems and machine learning applications.

**Organizer(s) :** Andre Milzarek, Zaiwen Wen

**Classification :** 90C06, 90C30

**Minisymposium Program :**

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00893 (1/3) : 1E @D501 [Chair: Andre Milzarek]

## [03305] An efficient skipping BFGS algorithm with nice Hessian correction properties

**Author(s) :** Yu-Hong Dai (AMSS)

**Abstract :** An efficient skipping BFGS algorithm is designed with nice Hessian correction properties. We analyze the skipping method from the perspective of improving quasi-Newton equations by operators and derive stronger quadratic termination properties. Global convergence and superlinear convergence results are established under classical assumptions. Numerical experiments illustrate the efficiency of the proposed method compared with the standard BFGS method.

## [02797] An Overview of Stochastic Quasi-Newton Methods for Large-Scale Machine Learning

**Author(s) :** Tiande Guo (University of Chinese Academy of Sciences)Yan Liu (Naikai University)Congying Han (University of Chinese Academy of Sciences)

**Abstract :** Numerous intriguing optimization problems arise as a result of the advancement of machine learning. Second-order algorithms have their typical advantages in dealing with highly nonlinear and ill-conditioning

part\_2

problems. This paper provides a review on recent developments in stochastic variants of quasi-Newton methods, which construct the Hessian approximations using only gradient information. We concentrate on BFGS-based methods in stochastic settings and highlight the algorithmic improvements that enable the algorithm to work in various scenarios. Future research on stochastic quasi-Newton methods should focus on enhancing its applicability, lowering the computational and storage costs, and improving the convergence rate.

## [02795] Riemannian Natural Gradient Methods

**Format :** Talk at Waseda University

**Author(s) :** Zaiwen Wen (Peking University)Jiang Hu (The Chinese University of Hong Kong)Ruicheng Ao (Peking University)Anthony Man-Cho So (The Chinese University of Hong Kong)Minghan Yang (Peking University)

**Abstract :** In this talk, we present a Riemannian natural gradient method for large-scale optimization problems on Riemannian manifolds. Such problems arise in various machine learning and signal processing applications. The notion of Fisher information matrix is extended from the Euclidean setting. We establish the almost-sure global convergence and local convergence of our proposed method under standard assumptions. Numerical experiments on applications arising from machine learning demonstrate the advantages of the proposed method over state-of-the-art ones.

## [04755] Newton-PMR: Newton Subspace Methods with Complexity Guarantees for Non-convex Optimization

**Format :** Talk at Waseda University

**Author(s) :** Yang Liu (University of Oxford)Andre Milzarek (The Chinese University of HThe Chinese University of Hong Kong, Shenzhen)Kong, Shenzhen)Fred Roosta (the University of Queensland)

**Abstract :** Recently, Newton-MR methods have been introduced for solving nonconvex unconstrained smooth optimization problems. Leveraging the inherent ability of the minimum residual (MINRES) inner solver to detect directions of nonpositive curvature (NPC), Newton-MR variants enjoy a variety of optimal complexity guarantees. However, the application of these methods to modern high-dimensional problems remains challenging. To address this, we present novel variants that incorporate certain dimensionality reduction techniques. In particular, our proposed methods are based on recent results that have shown that preconditioning MINRES with a positive semi-definite but singular preconditioner is in fact equivalent to solving a low-dimensional problem whose dimension corresponds to the nullity of the preconditioning matrix. Utilizing these dimensionality reduction properties of preconditioned MINRES, we present novel variants of Newton-MR, called Newton-PMR, which can be readily applied to high-dimensional problems, while achieving desirable complexity guarantees.

00893 (2/3) : 2C @D501 [Chair: Yu-Hong Dai]

## [02799] Real-time tool path planning using deep learning for subtractive manufacturing

**Author(s) :** Yi-Fei Feng (University of Chinese Academy of Sciences)Li-Yong Shen (University of Chinese Academy of Sciences)Hong-YU Ma (University of Chinese Academy of Sciences)Chun-Ming Yuan (Academy of Mathematics and Systems Sciences, CAS)Xin Jiang (University of Chinese Academy of Sciences)

**Abstract :** Tool path planning is a crucial factor of computer-aided design and manufacturing. To generate suitable tool paths, the previous methods bases on traditional optimization often take to a long computational time. To achieve real-time planning, we propose an efficient neural network-based direct tool path generating method, and the whole process only takes a few microseconds. As an auxiliary result, a new tool path dataset with confined scallop height is first established for tool path training.

## [02796] NeuroPrim: An Attention-based Model for Solving NP-hard Spanning Tree Problems

**Author(s) :** Yuchen Shi (University of Chinese Academy of Sciences)Congying Han (University of Chinese Academy of Sciences)Tiande Guo (University of Chinese Academy of Sciences)

**Abstract :** We define the Markov Decision Process (MDP) for general combinatorial optimization problems on graphs and propose NeuroPrim, a novel framework for reducing the action and state space using the technique of Prim algorithm, which is trained by REINFORCE to solve various spanning tree problems. We apply it to three difficult problems on Euclidean spaces, namely Degree-constrained Minimum Spanning Tree (DCMST) problem, Minimum Routing Cost Spanning Tree (MRCST) problem and Steiner Tree Problem in graphs (STP). Experimental part\_2

results on literature instances show that our model is able to outperform strong heuristics and obtain small optimality gaps up to 250 vertices. In addition, we find no significant degradation on problem instances as large as 1000, which demonstrates our model has strong generalization ability.

## [02832] Streaming Algorithms for Maximizing the Difference of Submodular Functions

**Author(s)** : Wenguo Yang Cheng LU (UCAS)Suixiang GAO (UCAS)

**Abstract** : In this paper, we study the problem of maximizing the Difference of two Submodular (DS) functions in the streaming model, where elements of the ground set arrive one at a time in an arbitrary order. We present one-pass streaming algorithms for both the unconstrained and cardinality-constrained problems. Our analysis shows that the algorithms we propose are able to produce solutions with provable approximation guarantees. To the best of our knowledge, this is the first theoretical guarantee for the DS maximization problem in the streaming model.

## [03350] Recursive Importance Sketching for Rank Constrained Least Squares

**Author(s)** : Xudong Li (Fudan University)Yuetian Luo (University of Wisconsin-Madison)Anru Zhang (Duke University)Wen Huang (Xiamen University)

**Abstract** : In this talk, we propose a new Recursive Importance Sketching algorithm for rank constrained least squares optimization (RISRO). As its name suggests, the algorithm is based on a new sketching framework, recursive importance sketching. Several existing algorithms in the literature can be reinterpreted under the new sketching framework and RISRO offers clear advantages over them. RISRO is easy to implement and computationally efficient, where the core procedure in each iteration is only solving a dimension reduced least squares problem. Different from numerous existing algorithms with locally geometric convergence rate, we establish the local quadratic-linear and quadratic rate of convergence for RISRO under some mild conditions. In addition, we discover a deep connection of RISRO to Riemannian manifold optimization on fixed rank matrices. The effectiveness of RISRO is demonstrated in two applications in machine learning and statistics: low-rank matrix trace regression and phase retrieval. Simulation studies demonstrate the superior numerical performance of RISRO.

00893 (3/3) : 2D @D501 [Chair: Tiande Guo]

## [03278] A semismooth Newton stochastic proximal point algorithm with variance reduction

**Format** : Talk at Waseda University

**Author(s)** : Andre Milzarek (The Chinese University of Hong Kong, Shenzhen)Fabian Schaipp (Technical University of Munich)Michael Ulbrich (Technical University of Munich)

**Abstract** : We present an implementable stochastic proximal point (SPP) method for a class of weakly convex, composite optimization problems. The proposed stochastic proximal point algorithm incorporates a variance reduction mechanism and the resulting SPP updates are solved using an inexact semismooth Newton framework. We establish detailed convergence results that take the inexactness of the SPP steps into account. Finally, numerical experiments are shown illustrating that SPP competes favorably with other state-of-the-art methods.

## [00897] Nonlinear and nonlocal models: analysis and numerics

**Session Time & Room** :

00897 (1/2) : 2C (Aug.22, 13:20-15:00) @E504

00897 (2/2) : 2D (Aug.22, 15:30-17:10) @E504

**Type** : Proposal of Minisymposium

**Abstract** : The focus of the minisymposium will be on different aspects of nonlocal operators including regularity and numerical analysis of solutions to equations driven by fractional and nonlocal operators. In the recent years nonlocal models showed effectiveness in describing phenomena involving different singularities. We aims to bring

part\_2

together leading experts and young researchers interested in nonlocality, in particular for nonlinear problems, including:

Numerics and Scientific Computing, Modeling and Applications, Analysis of Partial Differential Equations, Calculus of Variations.

**Organizer(s)** : Anna Kh.Balci, Abner J. Salgado

**Classification** : 65-00

**Minisymposium Program :**

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00897 (1/2) : 2C @E504 [Chair: Abner Salgado]

### [04670] Energy gap for nonlocal model

**Format** : Talk at Waseda University

**Author(s)** : Anna Kh. Balci (University of Bielefeld, Germany)

**Abstract** : The essential feature of many models with non-standard growth is the possible presence of Lavrentiev gap and related lack of regularity, non-density of smooth functions in the corresponding energy space. Finding assumptions for the presence of Lavrentiev phenomena is in particular important for regularity theory. We show that nonlocal and local-nonlocal models enjoy the presence of energy gap. We obtain the optimal conditions separating the regular case from the one with Lavrentiev gap for the different types of nonlocal and mixed local-nonlocal double phase models. The obtained conditions show the sharpness of resent regularity results for nonlocal double-phase problems.

### [04387] Kacanov Iteration

**Format** : Talk at Waseda University

**Author(s)** : Lars Diening (Bielefeld University)Anna Kh. Balci (Bielefeld University)Johannes Storn (Bielefeld University)

**Abstract** : The p-Laplace equation is one of the model equations for non-linear problems. Due to its non-linearity it is quite challenging to approximate its solution numerically in particular in the degenerate/singular case. Standard methods like gradient descent or Newton's method have significant problems to approximate the solution. We present an iterative, linear method that allows to solve the p-Laplace equation efficiently both for small and large exponents.

### [04258] Regularity results for fractional nonlocal equation with nonstandard growth and differentiability

**Format** : Talk at Waseda University

**Author(s)** : Jihoon Ok (Sogang University)

**Abstract** : We discuss on nonlocal problems with nonstandard growth and differentiability. In particular, we introduce local boundedness and Hölder continuity for nonlocal double phase problems and nonlocal problems with variable growth and differentiability, by identifying sharp assumptions on parameters and functions characterizing these nonlocal problems.

### [05242] BBM-type theorem for fractional Sobolev spaces with variable exponents

**Format** : Talk at Waseda University

**Author(s)** : Minhyun Kim (Hanyang University)

**Abstract** : A Bourgain–Brezis–Mironeanu-type theorem for fractional Sobolev spaces with variable exponents is established for sufficiently regular functions. We prove, however, that a limiting embedding theorem for these spaces fails to hold in general.

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00897 (2/2) : 2D @E504 [Chair: Anna Balci]

## [05189] Time fractional gradient flows: Theory and numerics

**Author(s)** : Abner J Salgado (University of Tennessee)Wenbo Li (Chinese Academy of Sciences)

**Abstract** : We develop the theory of fractional gradient flows: an evolution aimed at the minimization of a convex, lower semicontinuous energy, with memory effects. This memory is characterized by the fact that the negative of the (sub)gradient of the energy equals the so-called Caputo derivative of the state. We introduce the notion of energy solutions, for which we provide existence, uniqueness and certain regularizing effects. We also consider Lipschitz perturbations of this energy. For these problems we provide an a posteriori error estimate and show its reliability. This estimate depends only on the problem data, and imposes no constraints between consecutive time-steps. On the basis of this estimate we provide an a priori error analysis that makes no assumptions on the smoothness of the solution.

## [05258] Semiconvexity estimates for integro-differential equations

**Format** : Talk at Waseda University

**Author(s)** : Marvin Weidner (Universitat de Barcelona)

**Abstract** : The Bernstein technique is a classical tool to establish derivative estimates for solutions to a large class of elliptic and parabolic equations. It is based on the maximum principle applied to suitable auxiliary functions. We explain how the Bernstein technique can be extended to integro-differential equations. As an application, we establish semiconvexity estimates for solutions to the nonlocal obstacle problem, the optimal regularity of the solution and

the regularity of the free boundary. Based on a joint work with Xavier Ros-Oton and Damià Torres-Latorre.

## [03356] Numerics and Analysis for Multi-Term Time-Fractional Burgers-Type Equation

**Author(s)** : Neetu Garg (National Institute of Technology Calicut)RaviKanth A.S.V. (National Institute of Technology Kurukshetra India)

**Abstract** : We present numerics and analysis for multi-term time-fractional Burgers-type. The proposed scheme consists of  $L_2$  formula in time and exponential B-splines in space. We apply semi implicit approach for the nonlinear term  $u\partial_x u$ . We study stability using the Von-Neumann method. We also discuss the convergence analysis. We solve a few numerical examples to examine the efficiency of the numerical scheme. Comparisons with the recent works confirm the robustness of the proposed scheme.

## [04692] The Spatially Variant Spectral Fractional Laplacian: Analytical Aspects and Parameter Selection

**Format** : Online Talk on Zoom

**Author(s)** : Carlos Rautenberg (George Mason University)Andrea Ceretani (University of Buenos Aires)

**Abstract** : We consider a variational definition for the spatially variant (spectral) fractional Laplacian and study the well-posedness of the associated Poisson's equation. The state space for the elliptic problem relies on non-standard Sobolev spaces with weights that are not of Muckenhoupt-type. The increased regularity of solutions is established together with the effectiveness of the fractional operator as a regularization for inverse problems. The latter leads to the optimal selection of the fractional order in image reconstruction.

## [00908] Machine Learning and Data-Driven Applications using Geometric Integration

**Session Time & Room :**

00908 (1/2) : 2E (Aug.22, 17:40-19:20) @E817

00908 (2/2) : 3C (Aug.23, 13:20-15:00) @E817

**Type :** Proposal of Minisymposium

**Abstract :** Machine learning techniques are becoming increasingly prominent at solving complex dynamical systems and utilized in data-driven applications, such as inverse problems and model discovery. Yet, important geometric and physical structures have not traditionally been incorporated in such approaches, leading to loss of accuracy in long-term predictions. This minisymposium aims to bring together researchers from diverse groups to improve on machine learning techniques using ideas inspired by geometric integration.

**Organizer(s) :** Elena Celledoni, James Jackaman and Andy Wan

**Classification :** 68T07, 65P10, 37M15

**Minisymposium Program :**

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00908 (1/2) : 2E @E817 [Chair: James Jackaman]

### [03459] Geometric integration in machine learning

**Format :** Talk at Waseda University

**Author(s) :** James Jackaman (NTNU)

**Abstract :** Here, as a primer, we give an overview of the role geometric integration (of Hamiltonian systems) has played in the design of neural networks in recent years, with an emphasis on the stability guarantees this provides and the structures incorporated into the networks. Time permitting, we will move on to discuss how convolutional networks can be understood through finite differences and the theoretical benefits this comparison yields.

### [03490] Application of the Kernel Method to Learning Hamiltonian Equations

**Format :** Talk at Waseda University

**Author(s) :** Taisei Ueda (Kobe University)Takashi Matsubara (Osaka University)Takaharu Yaguchi (Kobe University)

**Abstract :** Recently, methods for learning Hamiltonian systems from data have attracted much attention. While the most methods are based on neural networks, neural networks have some drawbacks, such as the possibility of falling into a local optimum. In this talk, we propose a method based on the kernel method, thereby overcoming the problems.

### [03180] Structured neural networks and some applications

**Format :** Online Talk on Zoom

**Author(s) :** Davide Murari (Norwegian University of Science and Technology)Elena Celledoni (Norwegian University of Science and Technology)Brynjulf Owren (Norwegian University of Science and Technology)Ferdia Sherry (University of Cambridge)Carola-Bibiane Schönlieb (University of Cambridge)

**Abstract :** Neural networks have gained much interest because of their effectiveness in many applications related to high-dimensional function approximation problems. This success is often supported by experimental evidence, while the theoretical properties of these models need to be better understood. When one knows that the target function to approximate or the data being processed has some properties, it might be desirable to reproduce them in the neural network design. This talk presents a framework that makes ODEs and numerical methods work together to model neural networks having prescribed properties. Such an approach is supported by offering particular applications for data-driven modelling and image analysis.

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00908 (2/2) : 3C @E817 [Chair: Andy Wan]

### [02911] Auxiliary Functions as Koopman Observables

**Format :** Online Talk on Zoom

**Author(s) :** Jason John Bramburger (Concordia University)

**Abstract :** Many important statements about dynamical systems can be proved by finding scalar-valued auxiliary functions whose time evolution along trajectories obeys certain pointwise inequalities that imply the desired result. The most familiar of these auxiliary functions is a Lyapunov function to prove steady-state stability, but such functions can also be used to bound averages of ergodic systems, define trapping boundaries, and so much more. In this talk I will highlight a method of identifying auxiliary functions from data using polynomial optimization. The method leverages recent advances in approximating the Koopman operator from data, so-called extended dynamic mode decomposition, to provide system-level information without system identification. The result is a model-agnostic computational method that can be used to bound quantities of interest and develop optimal state-

dependent feedback controllers, while also functioning as a pre-conditioner to discovering accurate and parsimonious dynamical models from the data.

### [03401] Conservative Hamiltonian Monte Carlo

**Format :** Online Talk on Zoom

**Author(s) :** Geoffrey McGregor (University of Toronto) Andy Wan (University of Northern British Columbia)

**Abstract :** Markov Chain Monte Carlo (MCMC) methods enable us to extract meaningful statistics from complex distributions which frequently appear in parameter estimation, Bayesian statistics, statistical mechanics and machine learning. However, as the dimensionality of the problem increases, the convergence rate of MCMC sequences toward the stationary distribution slows down dramatically. This has led to the development of Hamiltonian Monte Carlo (HMC) [Duane et al. '87, Neal '93], to improve performance by solving a Hamiltonian system using symplectic numerical methods. However, modern high-dimensional applications still pose a significant challenge for HMC.

In this talk, we introduce Conservative Hamiltonian Monte Carlo (CHMC), which alternatively utilizes an energy-preserving numerical method, known as the Discrete Multiplier Method. We show that CHMC converges to the correct stationary distribution under appropriate conditions, and provide numerical examples showcasing improvements in convergence rates over HMC in high-dimensional problems. Furthermore, we also will present numerical results on Bayesian parameter estimation using CHMC.

### [03462] Model Reduction of Hamiltonian Systems based on Nonlinear Approximation Methods

**Format :** Talk at Waseda University

**Author(s) :** Silke Glas (University of Twente)

**Abstract :** In this talk we consider structure-preserving model reduction of Hamiltonian systems, such that the reduced model is again a Hamiltonian system. We extend the classical linear-subspace model reduction methods, where the best possible error is bounded by the Kolmogorov N-width to reduced models constructed via nonlinear approximations. In this talk, we will particularly choose symplectic quadratic embeddings as our nonlinear approximation function.

## [00911] Sparse Linear Solvers for Computational Science at Extreme Scales

**Session Time & Room :**

00911 (1/2) : 2C (Aug.22, 13:20-15:00) @E508

00911 (2/2) : 2D (Aug.22, 15:30-17:10) @E508

**Type :** Proposal of Minisymposium

**Abstract :** Sparse linear solvers are a basic component in the tool chain for scientific applications; solution of sparse linear systems is indeed one of the main computational kernels in physics-driven models for numerical simulation and, more recently, also in data-driven models. The current challenge of exascale requires to rethink numerical algorithms for efficient exploitation of heterogeneous massively parallel computers, embedding multi/many-core processors. In this MS we bring together some very active researchers in this field to discuss recent advancements in the development of highly scalable algorithms and software for solving and preconditioning sparse linear systems on modern high-end supercomputers.

**Organizer(s) :** Pasqua D'Ambra, Carlo Janna

**Classification :** 65F10, 65N55, HPC, Sparse Linear Algebra

**Minisymposium Program :**

00911 (1/2) : 2C @E508 [Chair: Pasqua D'Ambra]

## [02685] GMRES+AMG Navier-Stokes Pressure Projection Solvers with RAS and ORAS Smoothers

**Format :** Talk at Waseda University

**Author(s) :** Stephen Thomas (Advanced Micro Devices)Amik St-Cyr (Shell)Erika Strakova (IT4-innovations Ostrava)Allison Baker (National Center for Atmospheric Research)

**Abstract :** PeleLM is a Navier-Stokes combustion model. Extremely ill-conditioned problems arise for incompressible and reacting flows in the low Mach flow regime, particularly for cut-cell meshes in complex geometries, Prenter (2020) improved convergence rates for cut-cells by employing PCG-AMG with Schwarz smoothers. We combine ILU smoothers using iterative triangular solves with RAS and ORAS smoothers adapted to hypre for a new low-synch MGS-CGS GMRES. The iteration counts tend to remain constant and these smoothers reduce run times on many-core GPU's in the strong-scaling limit.

## [04144] Scalable domain decomposition solvers for cardiac reaction-diffusion cell-by-cell models

**Format :** Talk at Waseda University

**Author(s) :** Luca Franco Pavarino (University of Pavia)Ngoc Mai Monica Huynh (University of Pavia)Simone Scacchi (University of Milano)Fatemeh Chegini (Zuse Institute Berlin)Martin Weiser (Zuse Institute Berlin)

**Abstract :** Scalable preconditioners are constructed and analyzed for the iterative solution of composite Discontinuous Galerkin discretizations of reaction-diffusion systems of ordinary and partial differential equations arising in cardiac cell-by-cell models. These models lead to large-scale ill-conditioned discrete systems which have discontinuous global solutions across cells (subdomains) boundaries. A scalable convergence rate bound is proved for dual-primal cell-by-cell preconditioned operators. Numerical tests validate this bound and investigate its dependence on the discretization parameters.

## [04198] An immersed approach to fluid-structure-contact interaction

**Format :** Talk at Waseda University

**Author(s) :** Patrick Zulian (Università della Svizzera italiana)Maria Giuseppina Chiara Nestola (Università della Svizzera italiana)Rolf Krause (Università della Svizzera italiana)

**Abstract :** We presents an immersed technique for solving fluid-structure interaction (FSI) problems using dual Lagrange multipliers, which enables the resampling of discrete fields with standard matrix-vector multiplication within the nonlinear solution procedure. The fluid and structure are coupled in the overlapping volume, while different structures in contact are coupled on the surface using mortar-based techniques.

## [04292] Adapting Patch-based Relaxation to Generalized MHD Systems Within An Algebraic Multigrid Solver

**Format :** Talk at Waseda University

**Author(s) :** Raymond Tuminaro (Sandia National Laboratories)We discuss a multigrid algorithm for generalized magnetohydrodynamics (GMHD). This GMHD system has two different PDE terms that can each generate a large near null space, complicating the linear solution process. One expression contains the curl operator while the other arises from generalized Ohm's law. Michael Crockatt (Sandia National Laboratories)Graham Harper (Sandia National Laboratories)Allen Robinson (Sandia National Laboratories)

**Abstract :** We discuss multigrid solvers for generalized magnetohydrodynamics. This system has two PDE terms that each generate a large near null space. One expression contains the curl operator while the other arises from generalized Ohm's law. We propose a geometric multigrid algorithm based on Arnold-Falk-Winther relaxation. We then adapt the Rietzinger/Schoberl AMG scheme to the generalized system. We apply the resulting preconditioner to two test problems to illustrate its effectiveness.

## [04535] JXPAMG: an auto-tuning parallel AMG solver for extreme-scale numerical simulations

**Format :** Talk at Waseda University

**Author(s) :** Xiaowen Xu (IAPCM) Silu Huang (IAPCM) Xiaoqiang Yue (Xiangtan University) Runzhang Mao (IAPCM)

**Abstract :** JXPAMG is a parallel algebraic multigrid (AMG) solver for solving the extreme-scale sparse linear systems on modern supercomputers. It is designed follows the auto-tuning mechanisms allow JXPAMG to use different AMG strategies for different application features and architecture features, and thereby JXPAMG becomes aware of changes in these features. This talk introduces the algorithms, implementation techniques, auto-tuning mechanisms and applications of JXPAMG.

## [04594] PSCTOOLKIT: Parallel Sparse Computation Toolkit

**Format :** Talk at Waseda University

**Author(s) :** Fabio Durastante (University of Pisa) Pasqua D'Ambra (Institute for Applied Computing (IAC)-National Research Council of Italy (CNR)) Salvatore Filippone (University of Rome "Tor Vergata")

**Abstract :** In this talk, we will describe a software framework for solving large and sparse linear systems on hybrid architectures, from small servers to high-end supercomputers, embedding multi-core CPUs and Nvidia GPUs. The framework has a tripartite modular structure, which separates basic functionalities for distributed sparse matrices and sparse matrix computations involved in Krylov methods, eventually exploiting multi-threading and CUDA-based programming models, from the setup and application of different types of preconditioners.

## [04611] Recent Developments in Two-level Schwarz Domain Decomposition Preconditioners in Trilinos

**Format :** Talk at Waseda University

**Author(s) :** Ichitaro Yamazaki (Sandia National Labs) Alexander Heinlein (Delft University of Technology (TU Delft)) Sivasankaran Rajamanickam (Sandia National Labs)

**Abstract :** Domain decomposition methods are used to build a class of effective parallel solvers for sparse linear systems arising from the discretization of partial differential equations. FROSCh is a software package, which implements GDSW type Two-level Schwarz Domain Decomposition preconditioners in Trilinos. In this talk, we present several recent developments made in FROSCh.

## [05152] Preparing Algebraic Multigrid Solvers in hypre for Exascale Computers

**Format :** Talk at Waseda University

**Author(s) :** Rui Peng Li (LLNL)

**Abstract :** The emerging exascale computers provide opportunities to perform much larger scale simulations to obtain more accurate solutions than ever before. The increasing complexities of heterogeneous accelerators on such platforms have made the development of sparse linear solvers challenging to achieve high performance. In this talk, we will discuss the porting strategies, new developments and performance optimizations of the multigrid solvers in hypre in preparation for the exascale computers with the results from real application codes.

# [00913] Geometric Mechanics and Related Topics

**Session Time & Room :**

00913 (1/2) : 2D (Aug.22, 15:30-17:10) @G710

00913 (2/2) : 2E (Aug.22, 17:40-19:20) @G710

**Type :** Proposal of Minisymposium

**Abstract :** Geometric mechanics is a research branch of modern differential geometric formulation for Lagrangian and Hamiltonian systems in mechanics, including related dynamical systems theory such as Hamiltonian bifurcations. Through the breakthrough of the famous symplectic reduction by Marsden and Weinstein and others,

part\_2

the scope of the field has expanded from mathematics and physics towards numerical and data sciences. This minisymposium describes the overviews on the main streams of geometric mechanics, including geometric methods in fluids and thermodynamics, and bridges many contemporary related topics such as dynamical systems, numerical simulations, information geometry, and data sciences from the view point of geometric mechanics.

**Organizer(s)** : Daisuke Tarama, Hiroaki Yoshimura

**Classification** : 37Jxx, 37Kxx, 65Pxx, 70Fxx, 53Zxx

**Minisymposium Program :**

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00913 (1/2) : 2D @G710 [Chair: Daisuke Tarama]

## [05487] Feedback Integrators for Mechanical Systems with Holonomic Constraints

**Format** : Talk at Waseda University

**Author(s)** : Joris Vankerschaver (Ghent University Global Campus)Dong Eui Chang (Korea Advanced Institute of Science and Technology)Matthew Perlmutter (Universidade Federal de Minas Gerais)

**Abstract** : We present a straightforward method for the numerical integration of the equations of motion of mechanical systems with holonomic constraints, to produce numerical trajectories that remain in the constraint set and preserve the values of constrained quantities. Our method only requires changes to the vector field and can be used in conjunction with any numerical integration scheme. This talk will describe the theoretical foundations of the method and compare its performance with other integrators.

## [04689] Geometric Integrators for Neural Symplectic Forms

**Format** : Talk at Waseda University

**Author(s)** : Yuhan Chen (Kobe University)Takashi Matsubara (Osaka University)Takaharu Yaguchi (Kobe University)

**Abstract** : The neural symplectic form is a deep physical model for general Hamiltonian systems in arbitrary coordinates. A primal application of deep physical models is physical simulations; however, when general numerical integrators are used for discretization, the physical properties are destroyed. Structure-preserving numerical methods are effective to address this problem. Typical integrators are symplectic integrators, which can be derived as variational integrators. In this study, we show that variational integrators are available for neural symplectic forms.

## [04691] Structure-Preserving Learning for GENERIC systems

**Format** : Talk at Waseda University

**Author(s)** : Baige Xu (Kobe University)Yuhan Chen (Kobe University)Takashi Matsubara (Osaka University)Takaharu Yaguchi (Kobe University)

**Abstract** : GENERIC (general equation for the non-equilibrium reversible-irreversible coupling) formulation is a key theory of non-equilibrium thermodynamics, with systems described by it having a unique geometric structure. We propose a neural network model that infers the equations of motion from observed data while preserving this geometric structure by applying the neural symplectic forms and introducing an equivalence relation between the models.

## [05507] A discretization of Dirac structures and Lagrange-Dirac dynamical systems

**Author(s)** : Hiroaki Yoshimura (Waseda University)Linyu Peng (Keio University)

**Abstract** : Various physical systems such as circuits, nonholonomic systems, as well as nonequilibrium thermodynamic systems can be formulated as a Lagrange-Dirac dynamical systems, in which an induced Dirac structure that is constructed by the canonical two-form and a distribution plays an essential role. In this talk, we show a discretization of such an induced Dirac structure and then we demonstrate how the associated discrete Lagrange-Dirac systems can be developed ,consistently with the discrete Lagrange-d'Alembert principle.

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00913 (2/2) : 2E @G710 [Chair: Hiroaki Yoshimura]

## [03436] Noether's conservation laws via the modified formal Lagrangians

**Format :** Talk at Waseda University

**Author(s) :** Linyu Peng (Keio University)

**Abstract :** Noether's theorem establishes a one-to-one correspondence between variational symmetries and conservation laws of variational differential equations. In this talk, we extend Noether's theorem to general differential equations by defining the modified formal Lagrangians. This allows us to construct conservation laws of non-variational differential equations using their symmetries. Worked examples will be provided.

## [05483] Harmonic exponential families on homogeneous spaces

**Format :** Talk at Waseda University

**Author(s) :** Koichi Tojo (RIKEN AIP)Taro Yoshino (The University of Tokyo)

**Abstract :** Exponential families play an significant role in the field of information geometry and are useful in Bayesian inference. Widely used families of probability measures, such as normal and gamma distributions can be considered as exponential families on homogeneous spaces with symmetry. Based on this observation, we presented a method to construct exponential families with symmetry using representation theory. In this talk, we will explain the method and its properties, illustrating them with examples.

## [04618] Symmetries and bifurcations of resonant periodic orbits in perturbed Rayleigh-Bénard convection

**Format :** Talk at Waseda University

**Author(s) :** Masahito Watanabe (Waseda University)Hiroaki Yoshimura (Waseda University)

**Abstract :** Rayleigh-Bénard convection is natural convection that appears in a fluid layer with heated bottom and cooled top planes. When Rayleigh number is set just above a critical number, velocity fields of Rayleigh-Bénard convection may oscillate slightly. In such oscillatory convection both stable and chaotic fluid transport may occur. In this talk we explore the global structures of periodic fluid transport in two-dimensional perturbed Rayleigh-Bénard convection in the perspectives of resonance, symmetry, and bifurcation.

## [05475] Geometric models in hydrodynamics

**Format :** Talk at Waseda University

**Author(s) :** Tudor Stefan Ratiu (Shanghai Jiao Tong University)Shanghai Jiao Tong University )

**Abstract :** In this talk the classical geometric formulation of hydrodynamics will be extended by the use of a momentum map with values in Cheeger-Simons differential characters. It will be shown that this extended momentum map admits topological conservation laws. Clebsch variables will be introduced for which the helicity takes integer values.

## [00915] The mathematics of quantum interaction models

**Session Time & Room :**

00915 (1/3) : 1C (Aug.21, 13:20-15:00) @D407

00915 (2/3) : 1D (Aug.21, 15:30-17:10) @D407

00915 (3/3) : 1E (Aug.21, 17:40-19:20) @D407

**Type :** Proposal of Minisymposium

**Abstract :** Research on quantum interaction models, describing the interaction of matter with light, has recently gained traction because of applications including quantum information science/technology and quantum computation. In contrast, despite the discovery of surprising relations with contemporary mathematical theory, including representation theory, geometry and number theory, the rich mathematical structure underlying these models has yet to be properly recognized. In this minisymposium we introduce the field and give an overview of recent results with a focus on the quantum Rabi model, the most fundamental model for light-matter interaction,

and discuss related models in quantum optics and solid-state physics.

**Organizer(s)** : Daniel Braak, Fumio Hiroshima, Cid Reyes Bustos, Masato Wakayama

**Classification** : 81V80, 81Q05, 47A10, 11M41, 81R40, Mathematical physics

**Minisymposium Program :**

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00915 (1/3) : 1C @D407 [Chair: Fumio Hiroshima]

## [03491] Quantum computation and its viewpoint from spectral zeta functions

**Format** : Talk at Waseda University

**Author(s)** : MASATO WAKAYAMA (NTT Institute for Fundamental Mathematics)

**Abstract** : We discuss the spectrum of the quantum interaction models such as the quantum Rabi models, non-commutative harmonic oscillators and their important derived models from the viewpoints of quantum computation and number theory via the corresponding heat kernels, partition functions and spectral zeta functions.

## [03218] New mathematics and machine learning applications from qubits and oscillators

**Format** : Talk at Waseda University

**Author(s)** : Sahel Ashhab (National Institute of Information and Communications Technology (NICT))

**Abstract** : I will present some of our studies on the physics of qubits and oscillators that produced interesting results that go into the realms of mathematics and computer science. In studying the dynamics of strongly driven qubits, we obtained a new approximation for Bessel functions. Our studies on the Landau-Zener problem, a hard problem that has a simple solution, inspired us to explore the use of symbolic regression to solve theoretical physics and mathematics problems.

## [03683] Design and optimization of fault-tolerant quantum computing

**Format** : Talk at Waseda University

**Author(s)** : Yasunari Suzuki (Nippon Telegraph and Telephone)

**Abstract** : To demonstrate scalable quantum computing, we need to suppress the high error rates of quantum devices. While they can be reduced with quantum error correction (QEC) technology, it requires large overheads on computing resources. Thus, optimization methods and co-design of hardware and software for fault-tolerant quantum computing are demanded. In this talk, I will explain the recent progress relevant to computer architecture and compiler optimization technologies based on the QEC framework.

## [04189] Energy spacing and time evolution for asymmetric quantum Rabi models

**Format** : Talk at Waseda University

**Author(s)** : Linh Thi Hoai Nguyen (Institute of Mathematics for Industry, Kyushu University)Cid Reyes Bustos (NTT IFM)Masato Wakayama (NTT Institute for Fundamental Mathematics)

**Abstract** : In this study, we describe the methods for numerical computations of the energy spacing distribution and time evolution for the asymmetric (or biased) quantum Rabi model (AQRM). The first several tens of thousands of eigenvalues are achieved by using the Truncated Hamiltonians method. From that, we observe the periodicity and symmetry of the consecutive energy spacing distribution with respect to the bias parameter. The time evolution is studied based on an explicit heat kernel formula.

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00915 (2/3) : 1D @D407 [Chair: Cid Reyes Bustos]

## [03826] The spectral problem in Hilbert spaces of analytic functions

**Format** : Online Talk on Zoom

**Author(s)** : Daniel Braak (University of Augsburg)

**Abstract** : In the standard Hilbert space, the spectral problem of Hamilton operators with one degree of freedom takes the form of a lateral connection problem for functions with diverging power series expansions. According to common lore, the solution would require to construct these functions on the whole real line which is usually impossible. It will

be demonstrated that this brute-force approach can be avoided by employing Hilbert spaces of analytic functions.

## [03426] The weak limit of renormalized Rabi Hamiltonian

**Format :** Talk at Waseda University

**Author(s) :** Fumio Hiroshima (Kyushu University)

**Abstract :** The weak limit of the renormalized Rabi Hamiltonian with a symmetry breaking term is investigated. It is shown that the spectral zeta function converges to the Riemann zeta function as the coupling constant goes to infinity. Furthermore the asymptotic behavior of the expectation of the number operator is also discussed.

## [03971] PT-Symmetric Quantum Rabi Model

**Format :** Talk at Waseda University

**Author(s) :** Murray Batchelor (Australian National University)

**Abstract :** We explore a PT-symmetric qubit coupled to a quantized light field. The model is solved analytically using the adiabatic approximation (AA) in the parameter regime of interest. We investigate the static and dynamic properties, using both the AA and numerical diagonalization. A series of exceptional points vanish and revive depending on the light-matter coupling strength. This talk is based on arXiv:2212.06586 with X. Lu, H. Li, J.-K. Shi, L.-B. Fan, V. Mangazeev and Z.-M. Li.

## [03421] Spectrum of the noncommutative harmonic oscillator and number theory

**Format :** Talk at Waseda University

**Author(s) :** Kazufumi Kimoto (University of the Ryukyus)

**Abstract :** The noncommutative harmonic oscillator (NCHO) is a system of differential equations defined by a certain matrix-valued operator, and it is connected to the quantum Rabi model via a confluent process in the Heun differential equation picture. In the talk, I will present number-theoretic aspects of the spectral zeta function of the NCHO, especially those arising from its special values (i.e. values at positive integers).

00915 (3/3) : 1E @D407 [Chair: Masato Wakayama]

## [03466] On the Weyl spectral counting function of certain semiregular global systems

**Format :** Online Talk on Zoom

**Author(s) :** Alberto Parmeggiani (University of Bologna)

**Abstract :** In this talk I will be discussing some recent work with Marcello Malagutti about the spectral asymptotics of certain global semiregular pseudodifferential systems. The class considered here contains important models such as the Jaynes-Cummings system, which is fundamental in Quantum Optics, but also models of geometric differential complexes over  $\mathbb{R}^n$ .

We give the asymptotics of the Weyl spectral counting functions in terms of the principal, semiprincipal and subprincipal symbols of the system, along with (time permitting) quasi-clustering properties of the spectrum.

## [03916] On The Spectral Zeta Function Of Second Order Semiregular Non-Commutative Harmonic Oscillators

**Format :** Online Talk on Zoom

**Author(s) :** Marcello Malagutti (University of Bologna)

**Abstract :** In this talk we give a meromorphic continuation of the spectral zeta function for semiregular Non-Commutative Harmonic Oscillators (NCHO). By “semiregular system” we mean a pseudodifferential systems with a step  $-j$

in the homogeneity of the  $j$ th-term in the asymptotic expansion of the symbol. As an application of our results, we first compute the meromorphic continuation of the Jaynes-Cummings (JC) model spectral zeta function. Then we compute the spectral zeta function of the JC generalization to a 3-level atom in a cavity. For both of them we show that it has only one pole in 1.

# [00917] High-dimensional regression and sampling

**Session Time & Room :**

00917 (1/3) : 3C (Aug.23, 13:20-15:00) @E507

00917 (2/3) : 3D (Aug.23, 15:30-17:10) @E507

00917 (3/3) : 3E (Aug.23, 17:40-19:20) @E507

**Type :** Proposal of Minisymposium

**Abstract :** The recovery of high-dimensional functions from point evaluations or more general linear measurements is a cornerstone of approximation theory and numerical analysis. While both are well-developed areas, the recent advances in learning theory and high-dimensional statistics sparked several new relations and tools for approximating functions. The research area hence has seen a quite remarkable synthesis of old and new results, especially in the context of nonlinear models such as neural networks and randomized techniques.

In this minisymposium we aim at highlighting recent developments of high-dimensional regression and sampling with modern applications in machine learning and function approximation.

**Organizer(s) :** Mario Ullrich, Andre Uschmajew

**Classification :** 65D40, 62J02, 62D99, 15A69, 65D15

**Minisymposium Program :**


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00917 (1/3) : 3C @E507 [Chair: André Uschmajew]

## [05486] Lattice-based algorithms for multivariate function approximation

**Format :** Talk at Waseda University

**Author(s) :** Frances Kuo (UNSW Sydney)

**Abstract :** This will be a talk on using lattices for multivariate function approximation.

## [05565] Efficient recovery of non-periodic multivariate functions via samples

**Format :** Talk at Waseda University

**Author(s) :** Nicolas Nagel (Chemnitz University of Technology)Tino Ullrich (Chemnitz University of Technology)Kai Lüttgen (Chemnitz University of Technology)Felix Bartel (Chemnitz University of Technology)

**Abstract :** Based on previous observations on function recovery from samples via Chebyshev polynomials, we introduce a periodization technique which preserves smoothness and thus, via known results for the periodic case, yields an efficient recovery algorithm for non-periodic functions. Together with deterministic subsampling algorithms we can prove, for the first time, near optimal bounds on the approximation error and support these claims with numerical experiments. This talk is based on work together with Felix Bartel, Kai Lüttgen and Tino Ullrich.

## [04593] Polynomial tractability for integrating functions with slowly decaying Fourier series

**Format :** Talk at Waseda University

**Author(s) :** Takashi Goda (The University of Tokyo)

**Abstract :** This talk is concerned with high-dimensional numerical integration problem. In this context, polynomial tractability refers to the scenario where the minimum number of function evaluations required to make the worst-case error less than or equal to a tolerance  $\varepsilon$  grows only polynomially with respect to  $\varepsilon^{-1}$  and the dimension  $d$ . For function spaces that are unweighted, meaning that all variables contribute equally to the norm of functions, there are many negative results known in the literature that exhibit the curse of dimensionality.

The aim of this paper is to show a contrasting result by introducing a non-trivial unweighted function space with absolutely convergent Fourier series that exhibits polynomial tractability with an explicit quasi-Monte Carlo rule.

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00917 (2/3) : 3D @E507 [Chair: Mario Ullrich]

## [04266] Weighted least-squares approximation in expected $L^2$ norm

**Format :** Talk at Waseda University

**Author(s) :** Matthieu Dolbeault (Sorbonne Université)Albert Cohen (Sorbonne Université)Abdellah Chkifa (Mohammed VI Polytechnic University)

**Abstract :** We investigate the problem of approximating a function in  $L^2$  with a linear space of functions of dimension  $n$ , using only evaluations at  $m$  chosen points. We improve on earlier results based on the solution to the Kadison-Singer problem, by using a randomized greedy strategy, which allows to reduce the oversampling ratio  $m/n$  and provides an algorithm of polynomial complexity.

## [05485] On the relation between adaptive and non-adaptive randomized sampling

**Format :** Talk at Waseda University

**Author(s) :** Stefan Heinrich (RPTU Kaiserslautern-Landau)

**Abstract :** Recently the author solved a long-standing problem of Information-Based Complexity: Is there a constant  $c > 0$  such that for all linear problems the randomized non-adaptive and adaptive  $n$ -th minimal errors can deviate at most by the factor  $c$ ? The analysis of vector-valued mean computation showed that the answer is negative.

In this talk we give a survey on this and related results concerning further aspects the problem.

## [05488] A multivariate Riesz basis of ReLU neural networks

**Format :** Talk at Waseda University

**Author(s) :** Cornelia Schneider (Friedrich-Alexander Universität Erlangen)Jan Vybiral (Czech Technical University)

**Abstract :** We consider the trigonometric-like system of piecewise linear functions introduced recently by Daubechies, DeVore, Foucart, Hanin, and Petrova. We provide an alternative proof that this system forms a Riesz basis of  $L_2([0,1]^d)$

**[0,1]<sup>d</sup>**

based on the Gershgorin theorem. We also generalize this system to higher dimensions  $d > 1$  by a construction, which avoids using (tensor) products. As a consequence, the functions from the new Riesz basis of  $L_2([0,1]^d)$

**[0,1]<sup>d</sup>**

can be easily represented by neural networks. Moreover, the Riesz constants of this system are independent of  $d$ , making it an attractive building block regarding future multivariate analysis of neural networks.

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00917 (3/3) : 3E @E507 [Chair: Mario Ullrich]

## [05533] On minimizing the training set fill distance in regression

**Format :** Talk at Waseda University

**Author(s) :** Paolo Climaco (Universität Bonn)Jochen Garcke (Universität Bonn & Fraunhofer SCAI)

**Abstract :** Machine learning regression methods leverage large datasets for training predictive models. However, using large datasets may not be feasible due to computational limitations or high labelling costs. Therefore, sampling small training sets from large pools of unlabelled data is essential to maximize performance while maintaining computational efficiency. In this work, we study a sampling approach aimed to minimize the fill distance of the selected set. We derive an upper bound for the maximum expected prediction error that linearly depends on the training set fill distance, conditional to the knowledge of data features. For empirical validation, we show that selecting a training by farthest point sampling significantly reduces the maximum prediction error, outperforming existing sampling approaches.

## [05514] Efficient training of Gaussian processes with tensor product structure

**Format :** Talk at Waseda University

**Author(s) :** Max Pfeffer (University of Goettingen) Josie König (Universität Potsdam) Martin Stoll (TU Chemnitz)

**Abstract :** We consider the special case of Gaussian process kernel learning where the covariance function is given by a sum of products of RBF kernels. For a given dataset, the parameters of the kernel are learned by minimizing the log marginal likelihood. Computing the log-determinant of the covariance matrix is prohibitive for large datasets or in high dimensions unless one exploits its low-rank tensor structure. We employ a stochastic trace estimation together with a Lanczos algorithm for TT-tensors (Tensor Trains). This allows us to break the curse of dimensionality and to perform a gradient-based optimization even in high dimensions.

## [05610] Tensor decompositions for high-dimensional kernel regression

**Author(s) :** Frederiek Wesel (Delft University of Technology) Kim Batselier (Delft University of Technology)

**Abstract :** Kernel machines provide a nonlinear extension to linear methods by projecting the data in a higher-dimensional feature space. When considering product kernels, the dimensionality of the feature space grows exponentially with the dimensionality of the data, limiting these methods to small-dimensional data. We lift this limitation by constraining the model weights to be a canonical polyadic decomposition of low rank. This allows us to derive a block coordinate descent algorithm which allows for the training of kernel machines under such constraint at a computational complexity which is linear both in the number of samples and in the dimensionality of the data, allowing to tackle both large-sampled and high-dimensional data.

## [05481] Optimal sampling for regression: from linear to nonlinear approximation

**Format :** Online Talk on Zoom

**Author(s) :** Anthony Nouy (Nantes Université - Centrale Nantes)

**Abstract :** We consider the approximation of functions in  $L^2$  from point evaluations, using linear or nonlinear approximation tools. For linear approximation, recent results show that weighted least-squares projections allow to obtain quasi-optimal approximations with near to optimal sampling budget.

This can be achieved by drawing i.i.d. samples from suitable distributions (depending on the linear approximation tool) and subsampling methods.

In a first part of this talk, we review different strategies based on i.i.d. sampling and present alternative strategies based on repulsive point processes that allow to achieve the same task with a reduced sampling complexity.

In a second part, we show how these methods can be used to approximate functions with nonlinear approximation tools, in an active learning setting, by coupling iterative algorithms and optimal sampling methods for the projection onto successive linear spaces. We particularly focus on the approximation using tree tensor networks, whose architectures allow for an efficient implementation of optimal sampling procedures within coordinate descent algorithms.

These are joint works with R. Gruhlke, B. Michel, C. Miranda and P. Trunschke

## [00919] Recent Advances in Hybridizable Discontinuous Galerkin Methods and Applications

**Session Time & Room :**

00919 (1/3) : 3E (Aug.23, 17:40-19:20) @E710

00919 (2/3) : 4C (Aug.24, 13:20-15:00) @E710

00919 (3/3) : 4D (Aug.24, 15:30-17:10) @E710

**Type :** Proposal of Minisymposium

**Abstract :** This minisymposium concentrates on the recent developments in numerical approximations to partial differential equations by hybridizable discontinuous Galerkin methods and other related schemes such as mixed methods, discontinuous Galerkin methods, and hybrid high-order methods. The scope of the talks is open to mathematical theory and applications of the methods in science and computational engineering, including the development of new hybridizable discontinuous Galerkin methods, Hamiltonian structure-preserving methods, grid adaptivity schemes, linear and nonlinear iterative methods, efficient implementations on emerging computer architectures, and robust shock capturing methods.

**Organizer(s) :** Jay Gopalakrishnan, Cuong-Ngoc Nguyen, Jaime Peraire, Manuel A. Sanchez

**Classification :** 65N30, 65M60, 65N55, 65N50, 65M22

**Minisymposium Program :**

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00919 (1/3) : 3E @E710

### [03033] A C0 interior penalty method for mth-Laplace equation

**Author(s) :** Weifeng Qiu (City University of Hong Kong)Huangxin Chen (Xiamen University)Jingzhi Li (Southern University of Science and Technology)

**Abstract :** In this paper, we propose a  $C^0$  interior penalty method for  $m$ th-Laplace equation on bounded Lipschitz polyhedral domain in  $R^d$ , where  $m$  and  $d$  can be any positive integers. The standard  $H^1$ -conforming piecewise  $r$ -th order polynomial space is used to approximate the exact solution  $u$ , where  $r$  can be any integer greater than or equal to  $m$ . Unlike the interior penalty method in Gudi and Neilan [IMA J. Numer. Anal. 31 (2011) 1734–1753], we avoid computing  $D^m$  of numerical solution on each element and high order normal derivatives of numerical solution along mesh interfaces. Therefore our method can be easily implemented. After proving discrete  $H^m$ -norm bounded by the natural energy semi-norm associated with our method, we manage to obtain stability and optimal convergence with respect to discrete  $H^m$ -norm.

### [03873] Output-Adaptive Hybridized Discontinuous Finite Elements for Efficient Flow Computations

**Author(s) :** Krzysztof Fidkowski (University of Michigan)

**Abstract :** Discontinuous Galerkin (DG) methods have enabled accurate computations of complex flowfields, yet their memory footprint and computational costs are large. Hybridized discontinuous Galerkin (HDG/EDG) methods reduce the number of globally-coupled degrees of freedom by decoupling elements and stitching them together through weak flux continuity. However, these methods have not risen to nearly the same level of popularity as DG, and in this work we outline reasons why and demonstrate benefits in an output-based adaptive setting.

### [04227] Towards boundary conditions for HDG methods for direct aeroacoustic computations

**Author(s) :** Philip Lukas Lederer (University of Twente)Jan Ellmenreich (TU Wien)

**Abstract :** We focus on direct aeroacoustic simulations using hybrid discontinuous Galerkin methods (HDG) for the approximation of the compressible Navier-Stokes equations. A crucial factor for accurate results is the proper handling of artificial boundary conditions, focusing on the reflectivity of the acoustic waves. We discuss various approaches such as LODI relations and extensions of characteristic Navier-Stokes boundary conditions (NSCBC) for HDG methods. Numerical results are presented and discussed in detail.

### [04312] Hybrid discontinuous Galerkin methods on multiple levels

**Author(s) :** Guido Kanschat (Heidelberg University)Peipei Lu (Soochow University)Roland Maier (University of Jena)Andreas Rupp (LUT University)

**Abstract :** Hybrid finite element schemes approximate the trace of an unknown solution to a partial differential equation on the mesh skeleton (the union of the faces in a mesh). Afterward, these schemes use this trace approximation to recover the primal and dual unknowns. This strategy has several advantages over standard finite elements, such as an enhanced order of convergence, smaller symmetric positive systems of linear equations, and preservation of physically meaningful quantities.

Virtually all of the available multilevel (multigrid and multiscale) techniques for finite elements exploit the fact that their test and trial spaces are nested. However, the test and trial spaces are not nested for hybrid finite elements because their main approximate lives on the mesh's skeleton, which grows with refinement. Thus, the major obstacle that blocks the way to practical multigrid methods comprises the construction of stable mesh transfer operators. Several recent works have addressed this issue by exchanging the hybrid formulation for a non-hybrid formulation in a preliminary step. Afterward, these approaches use the available multilevel strategies for non-hybrid finite elements.

We proceed differently and preserve the advantageous properties of hybrid finite elements on all mesh levels. To this end, we devise stable mesh transfer operators and provide relevant convergence results for our hybrid, multilevel finite elements. This approach allows us to use identical discretizations on all mesh levels (homogeneous strategy) instead of the heterogeneous methods that use different discretizations on different mesh levels.

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00919 (2/3) : 4C @E710

## **[04456] Combining finite element space-discretizations with symplectic time-marching schemes for linear Hamiltonian systems**

**Author(s)** : Manuel Sanchez (Pontificia Universidad Catolica de Chile)Bernardo Cockburn (University of Minnesota)Shukai Du (University of Wisconsin-Madison)

**Abstract** : We provide a short introduction to the devising of a special type of methods for numerically approximating the solution of Hamiltonian partial differential equations. These methods use Galerkin space-discretizations which result in a system of ODEs displaying a discrete version of the Hamiltonian structure of the original system. The resulting system of ODEs is then discretized by a symplectic time-marching method. This combination results in high-order accurate, fully discrete methods which can preserve the invariants of the Hamiltonian defining the ODE system. We restrict our attention to linear Hamiltonian systems, as the main results can be obtained easily and directly, and are applicable to many Hamiltonian systems of practical interest including acoustics, elastodynamics, and electromagnetism. After a brief description of the Hamiltonian systems of our interest, we provide a brief introduction to symplectic time-marching methods for linear systems of ODEs which does not require any background on the subject. We consider the case of finite-element space discretizations. The emphasis is placed on the conservation properties of the fully discrete schemes.

## **[04720] Multigrid for HDG**

**Author(s)** : Guosheng Fu (University of Notre Dame)Wenzheng Kuang (University of Notre Dame)

**Abstract** : We present optimal geometric and algebraic multigrid preconditioners for low-order and high-order HDG schemes for diffusion and Stokes problems. The algebraic multigrid is based on Jinchao Xu's auxiliary space preconditioning framework, while the geometric multigrid is based on the close connection between the lowest-order HDG scheme with the nonconforming Cruzeix-Raviart method. This is a joint work with Wenzheng Kuang from Notre Dame.

## **[04725] HDG method for elliptic interface problems and industrial application**

**Author(s)** : Masaru Miyashita Norikazu Saito (The University of Tokyo)

**Abstract** : We propose a hybridized discontinuous Galerkin (HDG) method to solve the interface problem for elliptic equations. We succeed in deriving optimal order error estimates in both the HDG norm and the L2 norm under low regularity assumptions for solutions such as  $u|_{\Omega_1} \in H^{1+s}(\Omega_1)$  and  $u|_{\Omega_2} \in H^{1+s}(\Omega_2)$  for some  $s \in (1/2, 1]$ . Numerical examples support our theoretical results. Then, we show an example of developing plasma equipment using the proposed method.

## **[04892] A C0 interior penalty method for mth-Laplace equation**

**Author(s)** : Weifeng Qiu (City University of Hong Kong)Huangxin Chen (Xiamen University)Jingzhi Li (SUSTech)

**Abstract** : I will talk about a C0 interior penalty method for the mth-Laplace equation.

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00919 (3/3) : 4D @E710

## [05082] Discontinuous Galerkin Methods for High Speed Flows

**Author(s)** : Ngoc Cuong Nguyen (Massachusetts Institute of Technology)Jaime Peraire (Massachusetts Institute of Technology)Jordi Perez (Massachusetts Institute of Technology)Loek Van Heyningen (Massachusetts Institute of Technology)

**Abstract** : We present discontinuous Galerkin (DG) methods for high-speed flows with particular focus on transition, turbulence, and shock capturing. We describe LDG, HDG, EDG methods and parallel iterative solvers with matrix-free preconditioners. We develop an adaptive viscosity regularization method for capturing shocks by minimizing the artificial viscosity field while enforcing smoothness constraints on the numerical solution. We present numerical results to demonstrate the DG methods and our shock capturing scheme on transonic, supersonic, and hypersonic flows.

## [00923] PDEs and variational computational methods in image processing, analysis and classification

**Session Time & Room :**

00923 (1/3) : 2C (Aug.22, 13:20-15:00) @G602

00923 (2/3) : 2D (Aug.22, 15:30-17:10) @G602

00923 (3/3) : 2E (Aug.22, 17:40-19:20) @G602

**Type** : Proposal of Minisymposium

**Abstract** : The minisymposium is devoted to a wide range of novel mathematical models and methods for image reconstruction, segmentation and PDEs based deep-learning classification, applied to time-lapse laser scanning microscopy, medical imagery, airborne and satellite optical and SAR data, arising in various fields of application like developmental and cell biology, medicine, nature protection and Earth biodiversity modelling and monitoring.

**Organizer(s)** : Karol Mikula, Serena Morigi

**Classification** : 35K55, 65K10, 65M08, 68U10, 68T05

**Minisymposium Program :**

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00923 (1/3) : 2C @G602 [Chair: Serena Morigi]

## [03551] Mathematical models and computational algorithms for 3D and 4D image processing in developmental biology and medicine

**Format** : Talk at Waseda University

**Author(s)** : Karol Mikula (Slovak University of Technology in Bratislava)

**Abstract** : We present mathematical models and numerical algorithms based on nonlinear advection-diffusion equations used for image filtering, segmentation and tracking in 3D+time microscopy images leading to automated reconstruction of the cell lineage tree during the first hours of embryogenesis. To achieve that goal, we discretize the nonlinear partial differential equations by the finite volume method, natural to image processing applications, and develop efficient and stable numerical schemes suitable for massively parallel computer architecture.

## [04223] Fractional graph Laplacian for image reconstruction

**Format** : Talk at Waseda University

**Author(s)** : Marco Donatelli (University of Insubria)Alessandro Buccini (University of Cagliari)

**Abstract** : We consider  $\ell^2 - \ell^q$  regularization with \$0

## [03561] Mathematical models for segmentation of Natura 2000 habitats in NaturaSat software

**Format :** Talk at Waseda University

**Author(s) :** Michal Kollár (Algoritmy:SK s.r.o. and Slovak University of Technology in Bratislava)Martin Ambroz (Slovak University of Technology in Bratislava)Aneta Alexandra Ozvat (Slovak University of Technology)Karol Mikula (Slovak University of Technology in Bratislava)Lucia Čahojová (Slovak Academy of Sciences)Mária Šibíková (Slovak Academy of Sciences)

**Abstract :** The contribution presents an overview of numerical methods and mathematical models designed for the NaturaSat software. The application allows botanists, environmentalists and nature conservationists across Europe to explore protected areas of Natura 2000 habitats using the Sentinel-2 optical data. The presented methods are designed for accurate area identification - semi-automatic and automatic segmentation of European protected habitats and monitoring of their spatio-temporal distribution and quality.

## [03205] NatNet - forward-backward diffusion classification tool

**Format :** Talk at Waseda University

**Author(s) :** Aneta Alexandra Ozvat (Slovak University of Technology)Karol Mikula (Slovak University of Technology in Bratislava)Michal Kollar (Slovak University of Technology)Martin Ambroz (Slovak University of Technology)Maria Sibikova (Slovak Academy of Sciences)Jozef Sibik (Slovak Academy of Sciences)

**Abstract :** The presentation introduces a novel method for PDE-based data classification using satellite optical data. The Natural Numerical Network (NatNet) is based on the numerical solution of the nonlinear forward-backward diffusion equation on a semi-complete directed graph. Partial differential equations on the directed graph are solved by a finite volume approach considering the balance of diffusion fluxes in the vertices of the graph. The presented natural numerical network is applied to Earth biodiversity modelling.

00923 (2/3) : 2D @G602 [Chair: Karol Mikula]

## [02834] Segmentation-based tracking of macrophages in microscopy videos

**Format :** Talk at Waseda University

**Author(s) :** Seol Ah Park (Slovak University of Technology in Bratislava)Tamara Sipka (University of Montpellier)Zuzana Kriva (Slovak University of Technology in Bratislava)Georges Lutfalla (University of Montpellier)Mai Nguyen-Chi (University of Montpellier)Karol Mikula (Slovak University of Technology in Bratislava)

**Abstract :** We propose an algorithm to achieve automatic cell tracking in macrophage videos.

First, we design a segmentation method employing space-time filtering, local Otsu's threshold, and the SUBSURF method.

Then, the partial trajectories are extracted when segmented cells overlap in time. Finally, the extracted trajectories are linked by considering their direction of movement. The automatic tracking achieved 97.4% of accuracy for macrophage data under challenging situations, feeble fluorescent intensity, irregular shapes, and motion of macrophages.

## [02927] Model-aware learning for super-resolution in fluorescence microscopy

**Format :** Talk at Waseda University

**Author(s) :** Luca Calatroni (CNRS)

**Abstract :** In this talk, I will present image super-resolution approaches for fluorescence microscopy applications based on the use of combined model-based and data-driven learning methods. Namely, I will show how generative adversarial training and plug-and-play learning methods can be effectively used as new paradigms for obtaining precise reconstructions with guarantees beyond the use of purely model-based approaches. Numerical results on both simulated and challenging real-world data will be presented.

## [02833] Macrophages trajectories smoothing by evolving curves

**Format :** Talk at Waseda University

**Author(s) :** Giulia Lupi (Slovak University of Technology in Bratislava) Karol Mikula (Slovak University of Technology in Bratislava) Seol Ah Park (Slovak University of Technology in Bratislava)

**Abstract :** We present a mathematical model and numerical method based on evolving open-plane and 3D curve approach in the Lagrangian formulation. The model contains three terms: the curvature term, the attracting term, and the tangential redistribution. We use the flowing finite volume method to discretize the advection-diffusion partial differential equation. We present results for macrophage trajectory smoothing and define a method to compute the cell velocity for the discrete points on the smoothed curve.

## [02718] Limited memory restarted lp-lq minimization methods using generalized Krylov subspaces

**Format :** Talk at Waseda University

**Author(s) :** Alessandro Buccini (University of Cagliari) Lothar Reichel (Kent State University)

**Abstract :** Regularization of certain linear discrete ill-posed problems, as well as of certain regression problems, can be formulated as large-scale, possibly nonconvex, minimization problems, whose objective function is the sum of the p-th power of the lp-norm of a fidelity term and the q-th power of the lq-norm of a regularization term, with  $0 < p, q \leq 2$ . We describe new restarted iterative solution methods that require less computer storage and execution time than the methods described by [Huang et al., Majorization-minimization generalized Krylov subspace methods for lp-lq optimization applied to image restoration. BIT (2017)]. The reduction in computer storage and execution time is achieved by periodic restarts of the method. Computed examples illustrate that restarting does not reduce the quality of the computed solutions.

00923 (3/3) : 2E @G602 [Chair: Cancelled]

# [00924] Calibration and Validation of Mathematical Models for Biological Systems

**Session Time & Room :**

00924 (1/2) : 3C (Aug.23, 13:20-15:00) @A512

00924 (2/2) : 3D (Aug.23, 15:30-17:10) @A512

**Type :** Proposal of Minisymposium

**Abstract :** The advent of big data in biology offers many new challenges and opportunities. In this minisymposium, we will discuss advances in calibration and validation of biologically-driven mathematical models, spanning biological applications such as cancer, symbiosis, and circadian rhythms. An equally diverse set of mathematical techniques will be discussed such as Bayesian approaches, agent-based parameter estimation, and machine learning approaches. The first session of our minisymposium will focus on challenges specific to cancer modeling such as leveraging population-level data while preserving inter-individual heterogeneity, while the second session of the minisymposium will focus on broader methodology development in inferring mechanisms from data.

**Organizer(s) :** Lihong Zhao, Tracy Stepien, Erica Rutter

**Classification :** 92-10, 92B05, 92B20, 92C17, 92C42

**Minisymposium Program :**

00924 (1/2) : 3C @A512 [Chair: Lihong Zhao]

## [01710] Multiscale spatiotemporal reconstruction of single-cell genomics data

**Format :** Talk at Waseda University

**Author(s) :** Qing Nie (University of California, Irvine)

**Abstract :** Cells make fate decisions in response to dynamic environments, and multicellular structures emerge from multiscale interplays among cells and genes in space and time. The recent single-cell genomics technology provides an unprecedented opportunity to profile cells. However, those measurements are taken as static snapshots of many individual cells that often lose spatial information. How to obtain temporal relationships among cells from such measurements? How to recover spatial interactions among cells, such as cell-cell communication? In this talk I will present our newly developed computational tools that dissect transition properties of cells and infer cell-cell communication based on nonspatial single-cell genomics data. In addition, I will present methods to derive multicellular spatiotemporal pattern from spatial transcriptomics datasets. Through applications of those methods to systems in development and regeneration, we show the discovery power of such methods and identify areas for further development for spatiotemporal reconstruction of single-cell genomics data.

## [01731] Integrating quantitative MRI with computational modeling to predict the response of breast cancers to neoadjuvant therapy

**Format :** Online Talk on Zoom

**Author(s) :** Thomas Yankeelov (The University of Texas at Austin)Chase Christenson (The University of Texas at Austin)Casey Stowers (The University of Texas at Austin)Reshma Patel (The University of Texas at Austin)Chengyue Wu (The University of Texas at Austin)

**Abstract :** We will discuss how magnetic resonance imaging data (MRI) can initialize and constrain mathematical models describing cancer proliferation, migration/invasion, vascular status, and drug-related growth inhibition and cell death. More specifically, we will focus on 1) incorporating patient-specific MRI data into biology-based mathematical models, and 2) optimizing outcomes via patient-specific digital twins in breast cancer. The long-term goal is to provide a rigorous methodology that allows for optimizing therapeutic interventions on a patient-specific basis.

## [04716] Deep Hybrid Modeling of Neuronal Dynamics using Generative Adversarial Networks

**Format :** Online Talk on Zoom

**Author(s) :** Casey Diekman (New Jersey Institute of Technology)Soheil Saghafi (New Jersey Institute of Technology)

**Abstract :** Mechanistic modeling and machine learning methods are powerful techniques for approximating biological systems and making accurate predictions from data. However, when used in isolation these approaches suffer from distinct shortcomings: model and parameter uncertainty limit mechanistic modeling, whereas machine learning methods disregard the underlying biophysical mechanisms. To address these shortcomings, we build Deep Hybrid Models (DeepHMs) that combine deep learning with mechanistic modeling to identify the distributions of mechanistic modeling parameters coherent to the data. We employed DeepHM to identify which ionic conductances are responsible for the altered excitability properties of CA1 pyramidal neurons in mouse models of Alzheimer's disease.

## [03082] Gene regulatory network dynamics in single cells

**Format :** Online Talk on Zoom

**Author(s) :** Adam L MacLean (University of Southern California)Megan Rommelfanger (University of Southern California)

**Abstract :** Single-cell genomics offer unprecedented resolution with which to study cell fate decision-making. We present new tools to infer gene regulatory networks (GRNs) controlling cell fate decisions and model their multiscale dynamics. We introduce popInfer, single-cell multi-modal GRN inference via regularized regression, and demonstrate its potential for network discovery. We develop a single-cell resolved multiscale model coupling cell-cell communication with gene regulatory network dynamics, with which we discover a profound role for cell-cell communication in hematopoiesis.

## [02727] The role of bacterial chemotaxis in microbial symbiosis

**Format :** Online Talk on Zoom

**Author(s) :** Douglas Brumley (The University of Melbourne)

**Abstract :** Bacterial motility, symbioses, and marine nutrient cycling unfold at the scale of individual microbes, and are inherently dynamic. In this talk, I will outline how iteratively combining video-microscopy, image processing and mathematical modelling can resolve dynamic microscale processes which underpin the ecology of microbes. I will also demonstrate how the highly-resolved processes at the scale of individual cells can be connected to bulk measurements at the population-level through calibrated mathematical models.

## [04509] Multi-scale modelling of the uterus and the 12 Labours project

**Format :** Online Talk on Zoom

**Author(s) :** Alys Rachel Clark (University of Auckland)Shawn Means (University of Auckland)Claire Miller (University of Auckland)Mathias Roesler (University of Auckland)Amy Garrett (University of Auckland)Leo Cheng (University of Auckland)

**Abstract :** Uterine contractions contribute to fertility, menstruation, and delivery of babies, and the uterus has unique properties compared to other smooth muscle organs (including extensive stretch in pregnancy without contraction). Here, I present cell-to-tissue models of the uterus which form part of the 12 Labours project. This project takes a data-driven and reproducible approach to modelling physiological systems, which aims to integrate models into clinical workflows and provide feedback to wearable devices that monitor the uterus.

## [02752] Bayesian discovery of mechanics and signaling during collective cell migration

**Format :** Online Talk on Zoom

**Author(s) :** Simon Martina Perez (Oxford)Ruth E. Baker (University of Oxford)

**Abstract :** Collective cell migration results from a complex interplay of cell-cell interactions and whole-tissue mechanics. Experimental data enables Bayesian inference to identify the role of mechanics and cell-cell interactions. While mathematical models can be identified with sufficiently detailed data, the relationship between observation noise and uncertainty in the learned models remains unexplored. We explore how to combine data sets to quantify uncertainty, and draw mechanistic conclusions about the underlying biophysical process in morphogenesis and cancer invasion.

## [05213] PIEZO1 regulates cellular coordination during collective cell migration

**Format :** Talk at Waseda University

**Author(s) :** Jinghao Chen (University of California, Irvine)Jesse Holt (University of California, Irvine)Beth Evans (University of California, Irvine)John Lowengrub (University of California, Irvine)Medha Pathak (University of California, Irvine)

**Abstract :** The mechanically-activated ion channel PIEZO1 was recently identified to play an inhibitory role during wound healing. Through an integrative experimental and mathematical modeling approach, we elucidate PIEZO1's contributions to keratinocyte collective migration, an essential component of the healing process. Here, through a 2D-multiscale model of wound closure which links observations at both the single and multicell scales, and subsequent experimental validation, we identify cell directionality as being impacted by PIEZO1 activity during wound closure.

## [00932] Some recent advances on time-modulated metamaterials

**Session Time & Room :**

00932 (1/2) : 5B (Aug.25, 10:40-12:20) @D404

00932 (2/2) : 5C (Aug.25, 13:20-15:00) @D404

**Type :** Proposal of Minisymposium

**Abstract :** Time-modulated materials constitute the brand new class of metamaterials that is currently raising a huge interest in the mathematics, physics and engineering communities for their ability to achieve extreme wave phenomena. Indeed, by time modulating the properties (acoustic, optical, mechanical, etc.) of materials, one can, for instance, break reciprocity, achieve screening of parts of the domain by wave propagation, and reconfigure materials for optimization. The aim of this minisymposium is to bring together an interdisciplinary group of researchers to discuss the most recent results in the field and to favor interaction between theorists and experimentalists.

**Organizer(s) :** Kshiteej J. Deshmukh, Ornella Mattei

**Classification :** 78-xx, 74-xx, 35-xx

**Minisymposium Program :**

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00932 (1/2) : 5B @D404 [Chair: Prof. Ornella Mattei]

## [04433] Modeling Plasmons on Graphene with Time- and Space-Dependent Properties

**Format :** Talk at Waseda University

**Author(s) :** Fadil Santosa (Johns Hopkins University) Tong Shi (University of Minnesota)

**Abstract :** Graphene sheets are two-dimensional materials that are known to support plasmonic modes. The latter are electromagnetic waves which are concentrated near a surface and propagate along it. In graphene, these modes can exist on both sides of surfaces of the 2-D material. It has been shown that graphene sheets are effective in its ability to concentrate light, and for this reason, it is a candidate for photonic devices. In this work, we study graphene sheets which have time- and space-dependent properties. They are modeled as a flat conductive sheet with time- and space-dependent Drude weights. We show that in two dimensions, the governing equations can be reduced to a single 1-D time-dependent integro-partial-differential equation. The equation can be discretized and also solved approximately using perturbation arguments. We demonstrate the accuracy of the approximate solution and also show interesting behavior of the plasmons when the Drude weight is modulated temporarily and spatially.

## [05163] Analytical and FDTD Modelling of EM Wave Interacting with Time-Varying Media

**Format :** Talk at Waseda University

**Author(s) :** Debdeep Sarkar (Indian Institute of Science, Bangalore)

**Abstract :** First, we will focus on quasi-analytical ODE (ordinary differential equations) based methods to analyze velocity modulation imparted on EM (electromagnetic) waves interacting with infinitely extended time-varying medium. Later, we will examine EM wave interaction with finitely extended time-varying media using in-house Finite Difference Time Domain (FDTD) simulation methods. After critical observations on the generated reflection and transmission spectra of signals, we will comment on possible applications in next generation communication and Radar technologies.

## [04583] Using Time-Varying Systems to Challenge Fundamental Limitations in Electromagnetics and Photonics

**Format :** Online Talk on Zoom

**Author(s) :** Francesco Monticone (Cornell University)

**Abstract :** Time-varying systems offer opportunities for efficient electromagnetic and photonic devices, potentially surpassing various well-established theoretical limits, such as the Bode-Fano limit, the Chu limit, the Rozanov bound, delay-bandwidth limits, and others. At the same time, the characteristics of the temporal dimension create challenges and constraints that are unique to time-varying systems. In this talk, I will first review these opportunities and limitations, and will then discuss some of our recent research efforts in this area.

## [03155] Energy conserving temporal metasurfaces

**Format :** Talk at Waseda University

**Author(s) :** Kshiteej Jayendra Deshmukh (University of Utah) Graeme W Milton (University of Utah)

**Abstract :** Changing the microstructure properties of a space-time metamaterial while a wave is propagating through it, in general requires addition or removal of energy, which can be of exponential form depending on the type of modulation.

This limits the realization and application of space-time metamaterials. In this work we present non-linear energy conserving temporal interfaces which address this problem.

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00932 (2/2) : 5C @D404

## [00935] Applied mathematics in industry: Success stories of collaboration between academia and industry in Mexico

**Session Time & Room :**

00935 (1/2) : 3C (Aug.23, 13:20-15:00) @D515

00935 (2/2) : 3D (Aug.23, 15:30-17:10) @D515

**Type :** Proposal of Industrial Minisymposium

**Abstract :** The applied collaboration between educational institutions in mathematics and industry is complicated not only from a scientific and technological point of view but also due to intellectual property legislation, organization, response time, and confidentiality. This mini-symposium will present successful real cases of applying mathematics directly to technological development in Mexico and some ideas for achieving greater collaboration.

**Organizer(s) :** Ivete Sanchez Bravo, Giovana Ortigoza Alvarez, Yasmin Rios Solis

**Classification :** 90Bxx

**Minisymposium Program :**

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00935 (1/2) : 3C @D515 [Chair: Ivete Sanchez]

## [01598] Public Transportation in Mexico

**Format :** Online Talk on Zoom

**Author(s) :** Yasmin Rios Solis (Tecnológico de Monterrey)

**Abstract :** Mexican public transportation planning and operation need different mathematical models than the ones used in developed countries. Indeed, planning stages like timetables and frequency setting should be revisited weekly or even daily. I will present two case studies of companies in Mexico and the main points that differentiate the classical models in the scientific literature from the needed ones. In particular, we will talk about the timetabling problem together with the vehicle scheduling problem to minimize the number of unfulfilled trips. I will present the models, the real case, and computational experimentation.

## [01632] Successful cases of mathematical applications for business

**Format :** Talk at Waseda University

**Author(s) :** Ivete Sanchez-Bravo (Centro de Investigación en Matemáticas)

**Abstract :** Science and technology are two key elements for the development of all countries. The industrial sector seeks to apply frontier knowledge to generate value in its processes and products, so it needs a translation to apply it, in addition to having personnel trained in these topics.

This talk will present the results and successful partnerships between some Mexican and multinational companies, as well as some initiatives such as workshops for companies to encourage teamwork, organized by CIMAT with other institutions specifically in areas of Applied Mathematics, such as AI, Optimization, and Data Science.

## [01653] Statistical Methods for Natural Disaster Risk Assessment

**Format :** Online Talk on Zoom

**Author(s) :** Ramses H Mena (UNAM)

**Abstract :** The study and risk assessment of natural disasters are of crucial interest for every country. The ability to foresee potential losses are of paramount importance for emergency policies, prevention, reconstruction and risk transfer mechanisms. Using a case study with the Mexican Natural Disasters Fund (FONDEN), we will discuss the importance of statistical and probabilistic methodologies created to aid the insurance against natural disasters.

## [01743] Collaboration between SMM and mathematical professionals in the mexican industry

**Format :** Talk at Waseda University

**Author(s) :** Giovana Ortigoza Alvarez (Seguros Monterrey New York Life)

**Abstract :** The collaboration between mathematics graduates in Mexico and the Mexican Mathematical Society (SMM) has been of vital importance and a topic of interest in recent years.

Since 2016, through special sessions in the national congress that the (SMM) organizes each year, talks, panel discussion and workshops focused on the empowerment of mathematicians and the collaborations that can be developed in the private industry in Mexico are presented.

In this talk we will talk about this project.

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00935 (2/2) : 3D @D515 [Chair: Giovana Ortigoza]

## [01745] P&L Attribution and Risk Management

**Format :** Talk at Waseda University

**Author(s) :** Joyce Vega (Universidad Nacional Autónoma de México)

**Abstract :** In this session I will talk about the concept of profit and loss attribution in risk management as a predictive and explanatory model of financial market movements in investment portfolios through Taylor expansion, and associated concepts of risk factors as components of a price function of a financial instrument. Finally, I will also present an applied example of this model.

## [01753] Building an university-based knowledge transfer network for the financial sector: The case of Fin-ML

**Format :** Online Talk on Zoom

**Author(s) :** Manuel Morales (Université de Montréal)

**Abstract :** In 2017, the Fin-ML Network was created within the Université de Montréal with the goal of training the next generation of applied mathematicians and statisticians working at the intersection of data-science, machine learning, quantitative finance and business intelligence. In the past five years, it has become a knowledge transfer center fostering collaboration between industry and academia around data-centric value creation for businesses in the financial sector. This collaboration is now international as we have started partnering with the innovation ecosystem in two Mexican states. This talk will narrate this success story while showcasing some of the applied projects our researchers have been working on.

## [01912] Applied mathematics in industry: Success stories of collaboration between academia and industry in Mexico

**Format :** Online Talk on Zoom

**Author(s) :** Cipriano Arturo Santos (Tecnológico de Monterrey)

**Abstract :** The applied collaboration between educational institutions in mathematics and industry is complicated not only from a scientific and technological point of view but also due to intellectual property legislation, organization, response time, and confidentiality. This mini-symposium will present successful real cases of applying mathematics directly to technological development in Mexico and some ideas for achieving greater collaboration.

## [00936] Recent advances in applications for large-scale data assimilation and inverse problems.

**Session Time & Room :** 4E (Aug 24, 17:40-19:20) @E504

**Type :** Proposal of Minisymposium

**Abstract :** The development of algorithms for data assimilation (DA) and inverse problems (IPs) has been traditionally driven by very specific applications in engineering, medicine and the geosciences. However, algorithms that were initially tailored for geophysical data assimilation have now been used for solving tomographic inverse problems in engineering. Similarly, developments on imaging methods have been used for DA. This exchange has not only led to further algorithmic developments but also deeper theoretical insights. In this minisymposium we bring together experts on DA and IPs that work at the interface with applied sciences, with the aim of fostering knowledge transfer across disciplines

**Organizer(s) :** Svetlana Dubinkina, Marco Iglesias

**Classification :** 65-XX

**Minisymposium Program :**

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00936 (1/1) : 4E @E504 [Chair: Svetlana Dubinkina]

## [05372] Level-set parameterisations for Ensemble Kalman Inversion

**Format :** Talk at Waseda University

**Author(s) :** Marco Iglesias (University of Nottingham)

**Abstract :** We discuss a level-set approach to parameterise unknown interfaces and discontinuous properties with the Ensemble Kalman Inversion (EKI) framework for inverse problems. We demonstrate the applicability of this approach to solve various inverse problems where the unknown is a discontinuous property arising from the presence of an anomalous material/tissue. We will present numerical examples with applications to (i) non-destructive testing of composite materials, (ii) ground penetrating radar and (iii) magnetic resonance elastography.

## [05415] Data assimilation for estimating nonlinear dynamics in earthquakes

**Format :** Online Talk on Zoom

**Author(s) :** Femke Cathelijne Vossepoel (Delft University of Technology)Hamed Ali Diab-Montero (Delft University of Technology)Arundhuti Banerjee (Delft University of Technology)Celine Marsman (Utrecht University)Ylona van Dinther (Utrecht University)

**Abstract :** The highly nonlinear dynamics of earthquake sequences and the limited data availability make it very difficult, if not impossible, to forecast earthquakes. State- and parameter estimation with data assimilation can improve estimates and forecasts of earthquake sequences. We illustrate the challenges of data assimilation in earthquake simulation with a range of models using several ensemble data-assimilation methods, including the particle filter, the ensemble Kalman filter, the adaptive Gaussian mixture filter, and the particle flow filter.

## [05358] Analysis of a localized ensemble Kalman-Bucy filter with sparse observations

**Format :** Talk at Waseda University

**Author(s) :** Gottfried Hastermann (University of Potsdam)Jana de Wiljes (University of Potsdam)

**Abstract :** With large scale availability of precise real time data, their incorporation into physically based predictive models, became increasingly important. This procedure of combining the prediction and observation is called data assimilation. One especially popular algorithm of the class of Bayesian sequential data assimilation methods is the ensemble Kalman filter which successfully extends the ideas of the Kalman filter to the non-linear situation. However, in case of spatio-temporal models one regularly relies on some version of localization, to avoid spurious oscillations.

In this work we develop a-priori error estimates for a time continuous variant of the ensemble Kalman filter, known as localized ensemble Kalman-Bucy filter. More specifically we aim for the scenario of sparse observations applied to models from fluid dynamics and space weather.

## [05397] Edge-preserving inversion with $\alpha$ -stable priors

**Format :** Talk at Waseda University

**Author(s) :** Jarkko Suuronen (LUT University)Tomás Soto (LUT University)Neil Chada (Heriot Watt University)Lassi Roininen (LUT University)

**Abstract :** The  $\alpha$ -stable distributions are a family of heavy-tailed and infinitely divisible distributions that are well-suited as prior distributions to edge-preserving inversion in the context of (discretization of) infinite-dimensional

continuous-time statistical inverse problems. In this talk we present a new hybrid approximation method well-suited to the application of such priors.

## [00941] Numerical methods for Hamilton-Jacobi equations and their applications

### **Session Time & Room :**

- 00941 (1/4) : 3D (Aug.23, 15:30-17:10) @F402
- 00941 (2/4) : 3E (Aug.23, 17:40-19:20) @F402
- 00941 (3/4) : 4C (Aug.24, 13:20-15:00) @F402
- 00941 (4/4) : 4D (Aug.24, 15:30-17:10) @F402

### **Type :** Proposal of Minisymposium

**Abstract :** Hamilton-Jacobi equations arise both in modeling front propagation and in decision-making processes (optimal control & differential games). As a result, they have a broad range of applications including seismic imaging, robotic navigation, photolithography, transportation engineering, optimization of medical treatment policies, and data science. Practical usefulness of HJ-based approaches hinges on efficient and accurate numerical methods, which often need to handle anisotropy, degenerate diffusion, and possible discontinuity of viscosity solutions. High-dimensional problems and HJ-based inverse problems pose additional computational challenges. This mini-symposium will focus on recent advances in numerics for HJ PDEs and their innovative use in a variety of applications.

**Organizer(s) :** Samuel Potter, Alexander Vladimirsksy, Hasnaa Zidani

**Classification :** 49Lxx, 49Mxx, 65Nxx, 49Nxx, 86A22

### **Minisymposium Program :**

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- 00941 (1/4) : 3D @F402 [Chair: Samuel Potter]

## [01729] HJ equations in optimizing system-level performance objectives of Evolutionary Game Theory models

### **Format :** Talk at Waseda University

**Author(s) :** Alexander Vladimirsksy (Cornell University)

**Abstract :** Evolutionary Game Theory models time-dependent competitions of "types" or "strategies" in a population. EGT can be used to model the natural selection in biological systems or evolving behavioral patterns among humans. Controlling EGT-models to optimize some system-level performance measures can be accomplished through solving HJ equations. We illustrate this by optimizing drug therapies with an EGT-based model of cancer dynamics. Parts of this talk reflect joint work with Mark Gluzman, MingYi Wang, and Jake Scott.

## [02691] Maximizing the probability of desirable outcomes in Hamilton-Jacobi framework

### **Format :** Talk at Waseda University

**Author(s) :** MingYi Wang (Cornell University)

**Abstract :** We introduce new tools for robust stochastic control of indefinite-horizon processes. In particular, we maximize the probability of keeping the (random) cumulative cost under any specific threshold. Our approach yields a 2nd-order HJB equation and "threshold-aware" optimal policies recovered for all initial configurations and a range of threshold values. We illustrate this method using examples from drug therapy optimization and sailboat path-planning. Joint work with A. Vladimirsksy, J. Scott, and REU students at Cornell University.

## [03127] Data assimilation for the eikonal equation on a manifold

### **Format :** Talk at Waseda University

**Author(s) :** Jerome Fehrenbach (Institut de Mathematiques de Toulouse)Lisl Weynans (University of Bordeaux)

**Abstract :** We propose a method to determine the source(s) and principal direction of a front propagation on an anisotropic surface, from indirect nonlinear measurements. This model aims at describing the propagation of

electrical waves at the surface of the heart. The framework of variational data assimilation leads to minimize a quadratic cost-function on a manifold. The Gauus-Newton algorithm is implemented using the Exp<sub>x</sub> map on this manifold.

## [03171] Hamilton-Jacobi equations on graphs with applications to data depth and semi-supervised learning

**Format :** Talk at Waseda University

**Author(s) :** Jeff Calder (University of Minnesota)Mahmood Ettehad (Institute for Mathematics and its Applications (IMA))

**Abstract :** Shortest path graph distances are widely used in data science and machine learning, however, they can be highly sensitive to corruption in graph structures. In this talk we study a family of Hamilton-Jacobi equations on graphs called the p-eikonal equation. We show that p=1 is a provably robust distance-type function on a graph and converges in the continuum limit to a geodesic density weighted distance function. We present applications to data depth and semi-supervised learning.

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00941 (2/4) : 3E @F402 [Chair: Hasnaa Zidani]

## [03726] Neural networks for first order HJB equations and application to front propagation with obstacle terms

**Format :** Talk at Waseda University

**Author(s) :** Olivier Bokanowski (LJLL, University Paris Cité)Olivier Bokanowski (LJLL, University Paris Cité)Averil Prost (Insa Rouen)Xavier Warin (EDF)

**Abstract :** We propose deep neural network schemes for Bellman's dynamic programming principlefor some deterministic optimal control problems,corresponding also to some first-order Hamilton-Jacobi-Bellman equations with an obstacle term.We give an error analysis in an average norm, which is new in this deterministic context. We give several academic numerical examples on front propagation problems with obstacles in order to show the relevance of the approach.

## [03517] A system of of Hamilton-Jacobi equations characterizing geodesic centroidal tessellations

**Format :** Talk at Waseda University

**Author(s) :** Adriano Festa (Politecnico di Torino)

**Abstract :** We introduce a class of systems of Hamilton-Jacobi equations characterizing geodesic centroidal tessellations, i.e. tessellations of domains with respect to geodesic distances where generators and centroids coincide. Typical examples are given by geodesic centroidal Voronoi tessellations and geodesic centroidal power diagrams.

An appropriate version of the Fast Marching method on unstructured grids allows computing the solution of the Hamilton-Jacobi system and therefore the associated tessellations. We propose various numerical examples to illustrate the features of the technique.

## [04710] Tropical and multi-level numerical methods for solving optimal control problems

**Format :** Talk at Waseda University

**Author(s) :** Marianne Akian (Inria and CMAP, Ecole polytechnique)Stephane Louis Gaubert (INRIA and CMAP, Ecole polytechnique)Shanqing Liu (CMAP, Ecole polytechnique and Inria)

**Abstract :** We develop and study several numerical approximations and algorithms for computing the solution of Hamilton-Jacobi partial differential equations satisfied by the value function of deterministic optimal control problems over a finite dimensional space.

These algorithms combine tropical numerical method or fast-marching method, with a multi-level discretization in a neighborhood of the optimal trajectories. For regular problems, the complexity as a function of precision, can be as for a one-dimensional problem.

## [04939] Exploiting Hamilton-Jacobi-Bellman equations in the representation and evolution of conservative dynamics.

**Format :** Online Talk on Zoom

**Author(s) :** Peter Dower (University of Melbourne) William McEneaney (University of California San Diego)

**Abstract :** Connections between Hamilton's action principle and optimal control are explored in the representation and evolution of conservative dynamics. By associating these dynamics with a Hamilton-Jacobi-Bellman equation or its characteristic system, dynamic programming and verification results are used to construct a fundamental solution and solve inverse problems. On longer time horizons, where the action is not "least", analogous developments are shown to follow using a notion of "stationary" control. Various applications are highlighted.

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00941 (3/4) : 4C @F402 [Chair: Alexander Vladimirskey]

## [03669] Sparse-grid WENO fast sweeping methods for Eikonal equations

**Format :** Online Talk on Zoom

**Author(s) :** Zachary Miksis (University of Notre Dame) Yong-Tao Zhang (University of Notre Dame)

**Abstract :** Fixed-point WENO fast sweeping methods are a class of explicit iterative methods for efficiently solving steady-state hyperbolic PDEs. For multidimensional nonlinear problems such as Eikonal equations, high-order fixed-point WENO fast sweeping methods still require quite a large amount of computational costs. In this talk, I shall present our recent work on applying sparse-grid techniques, an effective approximation tool for multidimensional problems, to fixed-point WENO fast sweeping methods for reducing their computational costs.

## [03495] Efficient high frequency wave propagation with small sampling density

**Format :** Online Talk on Zoom

**Author(s) :** Songting Luo (Iowa State University) Qing Huo Liu (Duke University)

**Abstract :** In this talk, we will present a few approaches for simulating high frequency wave propagation with low sampling density. One approach is based on WKBJ approximation, which leads to Hamilton-Jacobi type equations for the phase and amplitude. Such equations will be solved efficiently by well-established schemes and their solutions will be used for building the wave. In order to resolve the difficulty of capturing the caustics in the WKBJ approximation, we will further transform the problem into a fixed-point iteration problem that can be solved by operator-splitting based pseudospectral methods, which leads to another approach. Both approaches have low sampling densities that ensure the efficiency, verified by numerical experiments.

## [03786] Data-Driven Learning Method for Optimal Feedback Control

**Format :** Online Talk on Zoom

**Author(s) :** Qi Gong (University of California, Santa Cruz)

**Abstract :** Computing optimal feedback controls for nonlinear systems generally requires solving Hamilton-Jacobi-Bellman (HJB) equations, which, in high dimensions, is a well-known challenging problem due to the curse of dimensionality. In this talk, we present a model-based data-driven method to approximate solutions to HJB equations for high dimensional nonlinear systems. To accomplish this, we model solutions to HJB equations with neural networks trained on data generated without any state space discretization. Training is made more effective and efficient by leveraging the known physics of the problem and generating training data in an adaptive fashion. We further develop different neural networks approximation structures to improve robustness during learning and enhance closed-loop stability of the learned controller.

## [03577] Leveraging Multi-time Hamilton-Jacobi PDEs for Certain Scientific Machine Learning Problems

**Format :** Online Talk on Zoom

**Author(s) :** Jerome Darbon (Brown University) Paula Chen (Brown University) Tingwei Meng (UCLA) Zongren Zou (Brown University) George Em Karniadakis (Brown University)

**Abstract :** We establish a novel theoretical connection between specific optimization problems arising in machine learning and the multi-time Hopf formula, which corresponds to a representation of the solution to certain multi-time HJ PDEs. Through this connection, we increase the interpretability of the training process of certain machine learning applications by showing that when we solve these learning problems, we also solve a multi-time HJ PDE and, by extension, its corresponding optimal control problem.

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00941 (4/4) : 4D @F402

## [00949] Optimal and Efficient Algorithms for Inverse Problems

**Session Time & Room :**

00949 (1/2) : 5C (Aug.25, 13:20-15:00) @E505

00949 (2/2) : 5D (Aug.25, 15:30-17:10) @E505

**Type :** Proposal of Minisymposium

**Abstract :** This minisymposium aims at bringing researchers to share their recent progress and to inspire new ideas in the solution of inverse problems and its applications. Talks will address modeling, and theoretical and computational aspects of numerical methods for solving inverse problems.

**Organizer(s) :** Malena Espanol, Rosemary Renaut

**Classification :** 65F22, 65R32

**Minisymposium Program :**


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00949 (1/2) : 5C @E505 [Chair: Malena Espanol]

## [05576] Geometric Scattering on Measure Spaces

**Format :** Online Talk on Zoom

**Author(s) :** Michael Perlmutter (Boise State University)

**Abstract :** Geometric Deep Learning is an emerging field of research that aims to extend the success of machine learning and, in particular, convolutional neural networks, to data with non-Euclidean geometric structure such as graphs and manifolds. Despite being in its relative infancy, this field has already found great success and is utilized by, e.g., Google Maps and Amazon's recommender systems. In order to improve our understanding of the networks used in this new field, several works have proposed novel versions of the scattering transform, a wavelet-based model of neural networks for graphs, manifolds, and more general measure spaces. In a similar spirit to the original scattering transform, which was designed for Euclidean data such as images, these geometric scattering transforms provide a mathematically rigorous framework for understanding the stability and invariance of the networks used in geometric deep learning. Additionally, they also have many interesting applications such as the analysis of single-cell data

## [02094] Variable Projection Methods for Solving Separable Nonlinear Inverse Problems

**Format :** Talk at Waseda University

**Author(s) :** Malena Espanol (Arizona State University)

**Abstract :** Variable projection methods are among the classical and efficient methods to solve separable nonlinear least squares problems. In this talk, I will introduce the variable projection method and its use to solve large-scale blind deconvolution problems.

## [03302] Doubly Noisy Kaczmarz

**Format :** Talk at Waseda University

**Author(s) :** Anna Ma (UC Irvine)ELHoucine Bergou ( Mohamed VI Polytechnic University (UM6P))Aritra Dutta (University of Southern Denmark)Soumia Boucherouite ( Mohamed VI Polytechnic University (UM6P))Xin Li (University of Central Florida)

**Abstract :** Large-scale linear systems,  $Ax=b$ , frequently arise in inverse problems. Often, these systems are noisy due to operational errors or faulty data-collection processes. In the past decade, the randomized Kaczmarz algorithm (RK) was studied extensively as an efficient iterative solver for such systems. However, the convergence study of RKA in the noisy regime is limited and considers measurement noise in the right-hand side vector,  $b$ . Unfortunately, in practice, that is not always the case; the coefficient matrix  $A$  can also be noisy. In this talk, we motivate and discuss the application of RK to doubly noise linear systems, i.e., linear systems with noise in both

the measurements and the measurement matrix. The presented work is a joint collaboration with El Houcine Bergou, Soumia Boucherouite, Aritra Dutta, and Xin Li.

## [02096] Geometric Scattering on Measure Spaces

**Format :** Online Talk on Zoom

**Author(s) :** Michael Perlmutter (UCLA)

**Abstract :** Geometric Deep Learning is an emerging field of research that aims to extend the success of machine learning and, in particular, convolutional neural networks, to data with non-Euclidean geometric structure such as graphs and manifolds. Despite being in its relative infancy, this field has already found great success and is utilized by, e.g., Google Maps and Amazon's recommender systems.

In order to improve our understanding of the networks used in this new field, several works have proposed novel versions of the scattering transform, a wavelet-based model of neural networks for graphs, manifolds, and more general measure spaces. In a similar spirit to the original scattering transform, which was designed for Euclidean data such as images, these geometric scattering transforms provide a mathematically rigorous framework for understanding the stability and invariance of the networks used in geometric deep learning. Additionally, they also have many interesting applications such as the analysis of single-cell data

00949 (2/2) : 5D @E505 [Chair: Malena Espanol]

## [03055] Conditional sampling via block-triangular transport maps

**Format :** Talk at Waseda University

**Author(s) :** Ricardo Baptista (California Institute of Technology)Nikola Kovachki (NVIDIA)Bamdad Hosseini (University of Washington)Youssef Marzouk (MIT)

**Abstract :** We present an optimal transport framework for conditional sampling of probability measures. Conditional sampling is a fundamental task of solving Bayesian inverse problems and generative modeling. Optimal transport provides a flexible methodology to sample target distributions appearing in these problems by constructing a deterministic coupling that maps samples from a reference distribution (e.g., a standard Gaussian) to the desired target. To extend these tools for conditional sampling, we first develop the theoretical foundations of block triangular transport in a Banach space setting by drawing connections between monotone triangular maps and optimal transport. To learn these block triangular maps, we will then present a computational approach, called monotone generative adversarial networks (MGANs). Our algorithm uses only samples from the underlying joint probability measure and is hence likelihood-free, making it applicable to inverse problems where likelihood evaluations are inaccessible or computationally prohibitive. We will demonstrate the accuracy of MGAN for sampling the posterior distribution in Bayesian inverse problems involving ordinary and partial differential equations, and probabilistic image in-painting.

## [02631] Efficient importance sampling for Bayesian inverse problems using tensor-trains

**Format :** Talk at Waseda University

**Author(s) :** Tiangang Cui (Monash University)Sergey Dolgov (University of Bath)Robert Scheichl (Heidelberg University)

**Abstract :** We propose an efficient importance sampling method for rare events in high-dimensional problems, by approximating the optimal importance distribution in a scalable way as the pushforward of a reference distribution under composition of order-preserving transformations based on tensor-train decompositions. By designing a ratio estimator that estimates the normalizing constant using a separate importance distribution, it applies also to Bayesian inverse problems. The efficiency and robustness are demonstrated numerically on high-dimensional problems constrained by differential equations.

## [02317] On structured linear measurements for tensor data recovery

**Format :** Talk at Waseda University

**Author(s) :** Elizaveta Rebrova (Princeton University)

**Abstract :** Data-oblivious measurements present an important branch of low-rank data compression and recovery techniques, frequently used in streaming settings and within iterative algorithms. Typically, linear data-oblivious measurements involve some version of a random sketch that preserves the geometric properties of the data. When data is tensorial, a special challenge is to create a sketch with a structure that reflects tensor structure: this way, it can work similarly to a dense random sketch matrix but require much less memory to store and can be applied more efficiently. I will talk about our and others -- including Tropp, Udell et al, De Lathauwer et al -- recently

part\_2

proposed streaming sketch-based approaches for computing low-rank Tucker approximations of large tensors. I will discuss our new generalized theoretical guarantees for proving their accuracy on full-rank and noisy data with high probability from a wide range of measurements.

## [00951] Steps Toward Robust and Stable Artificial Intelligence

### **Session Time & Room :**

00951 (1/2) : 3E (Aug.23, 17:40-19:20) @E818

00951 (2/2) : 4C (Aug.24, 13:20-15:00) @E818

**Type :** Proposal of Minisymposium

**Abstract :** Despite significant recent technological advances in Artificial Intelligence (AI), AI systems sometimes make errors and will continue making errors in the future, from time to time. AI errors are usually unexpected; sometimes they are also malicious with the potential to result in dramatic and tragic consequences.

Handling and understanding abstract properties of these errors and developing methods of defence against various attacks and instabilities in modern large-scale high-dimensional AI operating in high-dimensional non-stationary world requires appropriate mathematical methods and techniques. This mini-symposium focuses on discussing relevant mathematical machinery for the analysis and verification of AI robustness and stability.

**Organizer(s) :** Ivan Tyukin, Alexander N. Gorban, Desmond Higham

**Classification :** 68Txx, Artificial Intelligence

### **Minisymposium Program :**

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00951 (1/2) : 3E @E818 [Chair: Ivan Tyukin]

## [03569] Adversarial Ink: Componentwise Backward Error Attacks on Deep Learning

**Format :** Online Talk on Zoom

**Author(s) :** Des Higham (University of Edinburgh)Lucas Beerens (University of Edinburgh)

**Abstract :** Deep neural networks are capable of state-of-the-art performance in many classification tasks. However, they are known to be vulnerable to adversarial attacks---small perturbations to the input that lead to a change in classification. We address this issue from the perspective of backward error and condition number, concepts that have proved useful in numerical analysis. To do this, we build on the work of Beuzeville et al. (2021). In particular, we develop a new class of attack algorithms that use component-wise relative perturbations. Such attacks are highly relevant in the case of handwritten documents or printed texts where, for example, the classification of signatures, postcodes, dates or numerical quantities may be altered by changing only the ink consistency and not the background. This makes the perturbed images look natural to the naked eye. Such "adversarial ink" attacks therefore reveal a weakness that can have a serious impact on safety and security. We illustrate the new attacks on real data and contrast them with existing algorithms. We also study the use of a componentwise condition number to quantify vulnerability.

## [05048] On the extended Smale's 9th problem, phase transitions in optimisation and the limits of AI

**Format :** Talk at Waseda University

**Author(s) :** Alexander James Bastounis (Leicester University)

**Abstract :** Instability is the Achilles' heel of AI and a paradox, with typical training algorithms unable to recover stable neural networks (NNs). Hence the fundamental question: can one find algorithms that compute stable and accurate NNs? If not, what are the foundational barriers we encounter across machine learning? These questions are linked to recent results on the extended Smale's 9th problem, which uncovers new phase transitions in optimisation and yields barriers on the computation of NNs.

## [04061] Intrinsic dimensionality of real-life datasets in biomedicine and drug discovery

**Format :** Online Talk on Zoom

**Author(s) :** Andrey Zinov'yev (Evotec)

**Abstract :** Intrinsic dimensionality (ID) is the most essential characteristic of a multidimensional data point cloud which determines the reliability and stability of the application of all machine learning methods. We provide a toolbox for estimating ID, and we benchmark it using several hundreds of real-life datasets. We demonstrate how data ID affects the results of applying deep classifiers and generative data models in biomedicine and drug discovery domains that allow the user to judge the prediction robustness.

## [05037] Generalised hardness of approximation and hallucinations -- On barriers and paradoxes in AI for image reconstruction

**Format :** Online Talk on Zoom

**Author(s) :** Anders Hansen (University of Cambridge)

**Abstract :** AI techniques are transforming medical imaging with striking performance. However, these new methods are susceptible to AI generated hallucinations, the phenomenon where realistically looking artefacts are incorrectly added to the reconstructed image, causing serious concerns in the sciences. The basic question is therefore: can hallucinations be prevented? This question turns out to be linked to a newly discovered phenomenon in the foundations of computational mathematics: generalised hardness of approximation, demonstrating methodological barriers in AI.

00951 (2/2) : 4C @E818 [Chair: Alexander Bastounis]

## [03891] Stochastic Separation Theorems for making AI Safe, Adaptive, and Robust

**Format :** Talk at Waseda University

**Author(s) :** Ivan Y Tyukin (King's College London)Alexander N Gorban (University of Leicester)

**Abstract :** In this talk we discuss the issues around stability and robustness of modern AI systems to data and structure perturbations. We show that determining robust generalisation may involve computational costs which are exponential in the dimension of AI feature spaces. As a potential way to mitigate the issue we discuss a set of results, termed stochastic separation theorems, which could be used to efficiently “patch” instances of instabilities as soon as they are identified.

## [05438] Advancements in Autodiff

**Format :** Talk at Waseda University

**Author(s) :** Elizabeth Cristina Ramirez (Columbia University)

**Abstract :** The reliance of backpropagation and other gradient-based algorithms on derivative calculations is well-known. Automatic differentiation, a powerful computational tool that often remains overlooked, allows for the efficient computation of gradients, surpassing the limitations of numerical differentiation. In this presentation, we aim to provide a concise overview of the inner workings of autodiff, as implemented in frameworks like TensorFlow, PyTorch, and JAX. Moreover, we will shed light on recent developments that enhance stability and expedite convergence.

## [00952] Numerical methods for emerging flow problems in geosciences

**Session Time & Room :**

00952 (1/2) : 1C (Aug.21, 13:20-15:00) @E702

00952 (2/2) : 1D (Aug.21, 15:30-17:10) @E702

**Type :** Proposal of Minisymposium

**Abstract :** In recent years, various flow problems have emerged in geosciences, and they demand development in numerical methods to meet scientific research and industry application needs. Such problems are generally multiscale and multiphysics; they involve various phenomena at different spatial and temporal scales, and our capabilities to simulate the problems remain limited. An example problem is the 2010 Gulf of Mexico oil spill that started from a small-scale effluent jet at the bottom of the ocean and then migrated to water surfaces as floating film patches with huge horizontal sizes. These problems are beyond the reach of conventional approaches, and their simulation is challenging, and new methods have to be developed. This symposium provides researchers with a platform to present their algorithms and simulations for these flow problems, including porous media flows, atmosphere flows, ocean flows, ocean ecosystems, etc. The presenters will discuss encountered difficulties, possible approaches, and future directions. The symposium contains presentations on computational methods and simulation of actual industry problems.

**Organizer(s) :** Jose E. Castillo, Hansong Tang, Anne-Claire Bennis

**Classification :** 65M06

**Minisymposium Program :**

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00952 (1/2) : 1C @E702 [Chair: Hansong Tang]

## [03640] Non-stationary probabilistic tsunami hazard assessments incorporating the influence of tides and sea level rise

**Format :** Online Talk on Zoom

**Author(s) :** Ignacio Sepulveda (San Diego State University)

**Abstract :** Tides are often the largest source of sea levels fluctuations. Two probabilistic-tsunami-hazard-assessments (PTHA) methods are proposed to combine the tidal-phase uncertainty with other tsunami uncertainties. The first method adopts a Stochastic-Reduced Order-Model (SROM) producing sets of tidal phase samples to be used in tsunami simulations. The second method uses tsunami simulations with prescribed collocation-tidal-phases and probability distributions to model the uncertainty. The methods are extended to non-stationary-probabilistic-tsunami-hazard-assessments (nPThA), combining tsunamis, tides and sea level rise.

## [02149] A hybrid numerical method for dispersive multiphase porous media flows

**Format :** Online Talk on Zoom

**Author(s) :** Prabir Daripa (Texas A&M University, College Station)

**Abstract :** We discuss a recently developed model of multiphase multicomponent porous media flows in the context of shear-thinning polymer flooding. This model is based on Darcy's law, Buckley-Leverett equations and shear-thinning constitutive laws. A multiscale hybrid numerical method based on a combination of discontinuous finite element method, modified method of characteristics, and data driven strategies is developed to solve this model. We study effects of dispersion and shear-thinning on the advective transport of constituents like polymers.

## [01968] Ocean canyon dynamics modeled using Mimetic Curvilinear Coastal Ocean Model

**Format :** Talk at Waseda University

**Author(s) :** Jared Brzanski (San Diego State University)

**Abstract :** A 3D case study for Monterey Bay, CA, is performed to validate and demonstrate the capabilities of the Mimetic Coastal Ocean Model (MCCOM) model for simulating non-hydrostatic flows. The MCCOM model can resolve features such as stratified flows, internal bore formation, and strongly nonlinear internal wave processes inside the steep bathymetry of the Monterey Canyon system by implementing the model on a fully 3D curvilinear mesh.

## [01610] Hierarchical models for the numerical simulation of shallow water flows

**Format :** Talk at Waseda University

**Author(s) :** Julian Koellermeier (University of Groningen)

**Abstract :** We introduce hierarchical moment models as a flexible way to derive hierarchies of models for shallow flows. The new hierarchical models are based on an expansion of the velocity profile. The equations for the expansion coefficients constitute an hierarchical system. We will exemplify the hierarchical models for 1D and 2D

application cases including their analysis and the extension to complex fluids. We highlight runtime and accuracy improvements with respect to standard shallow water equations.

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00952 (2/2) : 1D @E702 [Chair: Jose E. Castillo]

### **[02375] A stability solver for nonlinear mountain waves**

**Format :** Talk at Waseda University

**Author(s) :** Craig Epifanio (Texas A&M University)Prabir Daripa (Texas A&M University)Kevin Viner (Naval Research Lab, Monterey)

**Abstract :** One of the primary sources of clear-air turbulence in the atmosphere is the breaking of internal gravity waves forced by topography, otherwise known as mountain waves. In the present work, the linear stability of nonlinear mountain waves is considered through the application of a steady-state Newton solver combined with a discretized large eigenvalue problem. The results show that mountain waves are subject to instability over a broader range of parameters than previously considered.

### **[02890] Coupling numerical solutions of NS and GFD equations for ocean flows**

**Format :** Talk at Waseda University

**Author(s) :** Hansong Tang (City College of New York)

**Abstract :** This talk discusses the integration of a solver of the Navier Stokes (NS) equations and a solver for the geophysical fluid dynamics (GFD) equations. In the integrated system, the NS solver is applied to local, fully 3D flow phenomena, and the GFD solver is adopted to simulate the background ocean flows. We will discuss the coupling methods and numerical experiments. The presentation will also discuss the difficulties and topics of future study.

### **[02177] A machine learning approach to phytoplankton productivity across the GoM**

**Format :** Talk at Waseda University

**Author(s) :** Bailey Armos (Texas A&M University)Shuang Zhang (Texas A&M University)Prabir Daripa (Texas A&M University)

**Abstract :** Although the hypoxia and algal bloom events seen within the Gulf of Mexico (GoM) have been largely linked to nitrogen loading from the Mississippi River, the nutrient inputs from smaller have been largely unexplored. In this study, we built machine learning models from coupled river-ocean data to better understand and quantify the chlorophyll content on multiple timescales in different regions of the GoM. Our study will help mitigation strategies in a changing coastal environment.

## **[00955] Incorporating Immune System and Heterogeneous Dynamics into Infectious Disease Modeling**

**Session Time & Room :**

00955 (1/3) : 3E (Aug.23, 17:40-19:20) @A512

00955 (2/3) : 4C (Aug.24, 13:20-15:00) @A512

00955 (3/3) : 4D (Aug.24, 15:30-17:10) @A512

**Type :** Proposal of Minisymposium

**Abstract :** Pathogen interactions with immune systems are dynamic. Modeling these nonlinear interactions has traditionally been a separate endeavor from modeling disease spread in a population. In the current environment of accelerating zoonotic spillovers, in which increasing numbers of pathogens are adapting to new hosts, habitats that include within-host innate and adaptive immune systems, as well as sequence-level data, should not be ignored. We bring together a diverse group of researchers to

address the resulting multilevel modeling challenges. The three sessions in this minisymposium will focus on:

1. vector-borne pathogens
2. Any Pathogen Transmission Mode
3. air- and water-borne pathogens

**Organizer(s)** : Julie Allison Spencer, Fabio Milner, Joel C. Miller

**Classification** : 92-10, Mathematical modeling or simulation for problems pertaining to biology

**Minisymposium Program :**

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00955 (1/3) : 3E @A512 [Chair: Julie Allison Spencer]

## [04516] Modelling vector-borne disease dynamics and the impact of new interventions

**Format** : Online Talk on Zoom

**Author(s)** : Ilaria Dorigatti (Imperial College London)

**Abstract** : In this seminar, I will present recent modelling studies developed to analyse the transmission dynamics of vector-borne diseases and to quantify the efficacy of a new dengue antiviral drug (JNJ-1802) from in-vitro and in-vivo experiments and a dengue vaccine candidate (TAK-003) using phase-3 clinical trial data. These models can help assess the population-level impact of novel control interventions across transmission settings. I will discuss current challenges as well as opportunities.

## [04353] Hierarchical model of West Nile virus incorporating spatio-temporal environmental effects

**Format** : Talk at Waseda University

**Author(s)** : Laura Albrecht (Colorado School of Mines)

**Abstract** : West Nile virus is primarily transmitted between mosquitoes and birds, with humans as incidental hosts. Climate change may increase the risk of human infections as climatic variables have been shown to accelerate mosquito development, biting rates, and the incubation period of the disease. We developed a spatio-temporal hierarchical SEIR model that incorporates environmental covariates related to climate change. We use a Bayesian paradigm to fit our model and to predict human cases.

## [04123] How genomic data can inform contact patterns in epidemiological models

**Format** : Talk at Waseda University

**Author(s)** : Julie Allison Spencer (Los Alamos National Laboratory) Emma Goldberg (Los Alamos National Laboratory) Sara Del Valle (Los Alamos National Laboratory)

**Abstract** : Infectious diseases threaten global health, as illustrated by the COVID-19 pandemic. Population-level models have been essential for understanding and anticipating impacts, but their ability to forecast outcomes accurately has been limited due to the rapid evolution of viruses and limited availability of parameters. Using sequenced SARS-CoV-2 genomes with associated age metadata, we inferred phylogenetic trees and used a birth-death branching model to understand the role of heterogeneous age structure on transmission pathways.

## [05574] Capturing heterogeneity: Differential effects of temperature on Culex mosquito vectors

**Format** : Talk at Waseda University

**Author(s)** : Sarah Moser (Los Alamos National Laboratory)

**Abstract** : Culex spp. mosquitoes are the primary transmission vectors for West Nile virus (WNV) worldwide. The differential effects of temperature on mosquito range, distribution, and abundance pose challenges for disease forecasting and mitigation. Current models often assume a single vector species; through our scoping review on thermal response for Culex mosquito life history traits, we show the need to implement real-world species heterogeneity and present a useful data resource for modelers.

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00955 (2/3) : 4C @A512 [Chair: Fabio Augusto Milner]

## [04150] Immunological variables as structure variables of epidemic models

**Format :** Talk at Waseda University

**Author(s) :** Fabio Augusto Milner (Arizona State University)

**Abstract :** We present some ways to structure epidemic models with infection and immune response as structure variables. The infected class is modeled using a divergence-form partial differential equation with the boundary conditions incorporating the new infections. Some theoretical results are derived, as well as some examples from HIV-infection. Open theoretical and numerical problems will be described.

## [01323] Approximations and parameter inference of stochastic models in infectious disease epidemiology

**Format :** Online Talk on Zoom

**Author(s) :** Wasiur KhudaBukhsh (University of Nottingham)

**Abstract :** In this talk, we will consider stochastic compartmental models in infectious disease epidemiology. We will discuss when the stochastic models agree with their deterministic counterparts in some limiting regimes and when one stochastic model can be approximated in some precise mathematical sense by another. We will also consider the problem of parameter inference of such systems using notions of dynamical survival analysis (DSA).

## [04927] Intelligent immunity: wet labs, fat data, and machine learning

**Format :** Online Talk on Zoom

**Author(s) :** Kaitlyn Martinez (Los Alamos National Laboratory)

**Abstract :** Developing a universal diagnostic is a long standing challenge. However, the human immune system is able to distinguish pathogens and mounts response quickly, perhaps acting as a guide for design of improved, more general diagnostic development. In collaboration with lab scientists, we use data from hundreds of experiments along with both machine learning and mechanistic models to show the potential for determining the presence of bacteria from markers of a human immune response.

## [03423] Why do most sexually transmitted infections not produce long-term immunity?

**Format :** Talk at Waseda University

**Author(s) :** Joel C Miller (La Trobe University)

**Abstract :** Diseases that are classified as "Susceptible-Infected-Recovered" (SIR) are unable to reinfect previously infected individuals. In small communities outbreaks are short-term and the disease is unable to persist. Long-term persistence of an SIR disease requires a large community or many connected small communities, so that new births replenish the susceptible community. The spread of sexually transmitted infections is heavily influenced by the significant heterogeneity of contact rates within the population. We will show that this increases the required "critical community size" for an SIR infection to persist in sexual transmission networks.

00955 (3/3) : 4D @A512 [Chair: Sara Del Valle]

## [04157] Basic concepts for the Kermack and McKendrick model with individual heterogeneity

**Format :** Talk at Waseda University

**Author(s) :** Hisashi Inaba (Tokyo Gakugei University)

**Abstract :** The main purpose of my talk is to provide a mathematical basis for the recent arguments and calculations triggered by COVID-19 based on the heterogeneous Kermack-McKendrick model. The basic epidemiological concepts such as basic reproduction number, effective reproduction number, herd immunity threshold and final size are rigorously formulated based on the Kermack-McKendrick model with individual heterogeneity. Furthermore, we discuss a systematic recipe to reduce the infinite-dimensional system to the finite-dimensional ODE system.

## [04524] Statistical analysis of global COVID-19 wave dynamics

**Format :** Talk at Waseda University

**Author(s) :** Jessica Stockdale (Simon Fraser University)

**Abstract :** Different countries around the world experienced vastly different COVID-19 pandemics, and in many cases the complex interplay of driving forces behind this remain unclear. Patterns of hybrid and partial immunity affect the ability of new variants to invade, and therefore must be understood to build insightful predictive models. I will present our work in statistically modelling the relative influence of immunity, demographic, social, and other factors on the size and timing of variant-driven COVID-19 waves.

## [03113] Will cross-immunity protect the community from COVID-19 variants?

**Format :** Online Talk on Zoom

**Author(s) :** Marina Mancuso (Arizona State University) Steffen Eikenberry (Arizona State University) Abba Gumel (University of Maryland, College Park)

**Abstract :** The emergence of SARS-CoV-2 variants threaten the efficacy of COVID-19 vaccines. Not only can variants be potentially more infectious than the wild-type strain, but they may also partially evade existing vaccines. A two-strain, two-group mechanistic mathematical model is designed to assess the impact of vaccine-induced, cross-protective efficacy of COVID-19 transmission in the United States. We present conditions for achieving vaccine-derived herd immunity and results from global sensitivity analysis under different transmissibility and cross-protection scenarios.

## [04936] SARS-CoV-2 variant transition dynamics are associated with vaccination rates, number of co-circulating variants, and convalescent immunity

**Format :** Talk at Waseda University

**Author(s) :** Sara Del Valle (Los Alamos National Laboratory)

**Abstract :** I will discuss a retrospective analysis that characterized differences in the speed, timing, and magnitude of 16 SARS-CoV-2 variant waves/transitions for 230 regions, between October 2020 and January 2023. Our results show associations between the behavior of an emerging variant and the number of co-circulating variants as well as demographics and vaccination rates. These results suggest the behavior of a variant may be sensitive to the immunologic and demographic context of its location.

## [00957] Mathematics of thin structures

**Session Time & Room :**

00957 (1/2) : 1C (Aug.21, 13:20-15:00) @G802

00957 (2/2) : 1D (Aug.21, 15:30-17:10) @G802

**Type :** Proposal of Minisymposium

**Abstract :** Many models in mechanics, physics and biology invoke thin structures and physical processes therein. With this minisymposium we intend to bring together mathematicians working on the modeling, mathematical analysis and numerics of such models. Topics of particular interest include variational models for mechanical thin films and rods, e.g., featuring wrinkling, prestrain, microstructure, dislocations and their numerical treatment.

**Organizer(s) :** Patrick Dondl, Stefan Neukamm

**Classification :** 35Qxx, 74B20

**Minisymposium Program :**

00957 (1/2) : 1C @G802 [Chair: Stefan Neukamm]

## [04690] A simple numerical approach for elastic rods

**Format :** Talk at Waseda University

**Author(s) :** Patrick Dondl (Albert-Ludwig-University Freiburg)

**Abstract :** We derive a discrete version of the Kirchhoff elastic energy for rods undergoing bending and torsion and prove Gamma-convergence to the continuous model. This discrete energy is given by the bending and torsion energy of an interpolating conforming polynomial curve and provides a simple formula for the bending energy depending in each discrete segment only on angle and adjacent edge lengths. For the liminf-inequality, we need to introduce penalty terms to ensure arc length parametrization in the limit. For the recovery sequence a discretization with equal euclidean distance between consecutive points is constructed. Particular care is taken to treat the interaction between bending and torsion by employing a discrete version of the Bishop frame. To obtain a local description of the energy without any restrictions on a reference configuration we employ a variant of parallel transport where the singularity for antiparallel directions of current and reference configuration is removed.

## [04525] A homogenized bending theory for prestrained plates

**Format :** Talk at Waseda University

**Author(s) :** Klaus Böhnlein (TU Dresden) Stefan Neukamm (TU Dresden) David Padilla-Garza (TU Dresden) Oliver Sander (TU Dresden)

**Abstract :** Nonlinear plate theory described the energy of an incompressible and inextensible thin elastic sheet. In this work, we show a general rigorous derivation of a generalization of such a model for non-euclidean plates with microheterogeneous structures. We also analyze the limiting energy in some examples and discover interesting and counter-intuitive phenomena.

## [01825] Variational Modeling of Stress-Driven Rearrangement Instabilities

**Format :** Talk at Waseda University

**Author(s) :** Paolo Piovano (Politecnico di Milano)

**Abstract :** Variational models in the context of the theory of stress-driven rearrangement instabilities are considered to describe the morphology of crystalline materials under stress due to the interaction with other adjacent materials. The existence and regularity of energy minimizers is discussed in various settings, from two to higher dimensions, and in the framework of a two-phase free-boundary problem by letting free also the contact interface with the other materials, both in its coherent and incoherent portions.

00957 (2/2) : 1D @G802 [Chair: Patrick Dondl]

## [04480] Numerical approximation of the deformation of thin plates

**Format :** Talk at Waseda University

**Author(s) :** Andrea Bonito (Texas A&M University) Diane Guignard (University of Ottawa) Angelique Morvant (Texas A&M University) Ricardo H Nochetto (University of Maryland) Shuo Yang (Yanqi Lake Beijing Institute of Mathematical Sciences and Applications)

**Abstract :** We study the elastic behavior of prestrained and bilayer plates which can undergo large deformations and achieve nontrivial equilibrium shapes. The mathematical model consists of a fourth order minimization problem subject to a nonlinear and nonconvex metric constraint. We introduce a numerical method based on discontinuous Galerkin finite elements for the space discretization and a discrete gradient flow for the energy minimization. We discuss the properties of the method and present several insightful numerical experiments.

## [01792] A reduced model for plates arising as low energy Gamma-limit in nonlinear magnetoelasticity

**Format :** Talk at Waseda University

**Author(s) :** Marco Bresciani (University of Erlangen) Martin Kružík (Czech Academy of Sciences)

**Abstract :** We investigate the problem of dimension reduction for plates in nonlinear magnetoelasticity. The model features a mixed Eulerian-Lagrangian formulation, as magnetizations are defined on the deformed set in the actual space.

We consider low-energy configurations by rescaling the elastic energy according to the linearized von Kármán regime.

First, we identify a reduced model by computing the  $\Gamma$ -limit of the magnetoelastic energy, as the thickness of the plate goes to zero. Then, we introduce applied loads given by mechanical forces and external magnetic fields and we prove that, under clamped boundary conditions, sequences of almost minimizers of the total energy converge to

minimizers of the corresponding energy in the reduced model.

Subsequently, we study quasistatic evolutions driven by time-dependent applied loads and a rate-independent dissipation. We prove that energetic solutions for the bulk model converge to energetic solutions for the reduced model and we establish a similar result for solutions of the approximate incremental minimization problem. Both these results provide a further justification of the reduced model in the spirit of the evolutionary  $\Gamma$ -convergence.

## [04118] A novel dimensional reduction for the equilibrium study of inextensional material surfaces Author links open overlay panel

**Format :** Talk at Waseda University

**Author(s) :** Eliot Fried (Okinawa Institute of Science and Technology)Yi-Caho Chen (University of Houston)Roger Fosdick (University of Minnesota)

**Abstract :** A general framework is developed for finding the equations describing the equilibrium of an inextensional material surface with arbitrary flat reference shape that is deformed by applying tractions or moments to its edge. Euler-Lagrange equations are derived, leading to a complete and definitive set of equilibrium equations, which are a system of ordinary-differential equations for the spatial directrix.

## [01343] Mesoscale modeling of systems of planar wedge disclinations and edge dislocations

**Format :** Talk at Waseda University

**Author(s) :** pierluigi cesana (kyushu university)

**Abstract :** Planar wedge disclinations are rotational mismatches at the level of the crystal lattice entailing a violation of rotational symmetry. Alongside dislocations, disclinations are observed in classes of Shape-Memory Alloys undergoing the austenite-to-martensite transformation and in crystal plasticity. In this talk, I will describe some recent results on the modeling of planar wedge disclinations and edge dislocations via an energy minimization principle. We model disclinations and dislocations as the solutions to minimum problems for isotropic elastic energies under the constraint of kinematic incompatibility. Our main result is the analysis of the energetic equivalence of systems of disclination dipoles and edge dislocations in the asymptotics of their singular limit regimes. The material of this talk is mainly based on a collaboration with Prof M. Morandotti & L. De Luca [ht  
tps://arxiv.org/abs/2207.02511](https://arxiv.org/abs/2207.02511)

## [00959] Numerical modeling and analysis in electromagnetic applications

**Session Time & Room :** 2C (Aug.22, 13:20-15:00) @E701

**Type :** Proposal of Minisymposium

**Abstract :** This mini-symposium presents numerical modeling, analysis and simulation using finite element method in the field of electromagnetism at various scales, from analyzing quantum mechanical effects to calculating the scattering of electromagnetic wave in free space. The Schrodinger-Poisson system of equations to calculate electron states in 3D hetero-structure will be discussed. Numerical modeling of display device will be presented and numerical analysis will be explored for microwave circuits. The electromagnetic vector wave scattering problem is solved to analyze the field characteristics in the presence of stealth platform. This mini-symposium also introduces several challenging issues in these applications and proposes their solutions.

**Organizer(s) :** Eunjung Lee

**Classification :** 65N30, 00A71, Numerical Analysis and Simulation

**Minisymposium Program :**

00959 (1/1) : 2C @E701

## [03708] Recent Advances in Finite Element Methods for Electromagnetic Analysis on Integrated Circuits

**Author(s)** : Woochan Lee (Incheon National University)

**Abstract** : The finite element method plays a significant role in the electromagnetic analysis of integrated circuits (IC) in electrical engineering. As IC structures constitute a very large-scale problem, the resources required for finite element modeling and analysis increase exponentially, making high-speed electromagnetic analysis an essential factor. This talk reviews recent trends in accelerating electromagnetic analysis, including the fundamental application of time- and frequency-domain finite element methods, high-speed techniques utilizing brick element characteristics, and parallel processing techniques.

## [03728] Forced field continuity condition of object interface for the vector wave equation

**Author(s)** : Hyesun Na (Yonsei University)

**Abstract** : Electromagnetic wave scattering problem is considered when perfect electric conductor is coated with several dielectric layers. Solving the scattering problem using finite element method requires huge number of degrees of freedom. Insufficient degrees of freedom may not be able to capture the information about abrupt changes in the interface. This work proposes to force a field continuity condition on the functional to overcome the difficulty.

## [03748] A three-dimensional NEGF development using finite element method in the presence of heterogeneous quantum dots

**Author(s)** : URANCHIMEG DORLIGJAV (Yonsei university )

**Abstract** : In this work, we propose an algorithm to calculate electron density and space charge effect in 3D nanoscale device containing heterogeneous quantum dots. We begin by formulating the nonequilibrium Green's function (NEGF) approach to calculate electron density and apply a nonlinear solver for Poisson equation using the finite element method.

## [04959] A Moving Mesh Method for Nano-Rod Electro-Osmosis

**Author(s)** : Richard James (Samsung Display)Jahoon Koo (Samsung Display)Sunyoung Oh (Samsung Display)Hyunguk Cho (Samsung Display)Sung-Chan Jo (Samsung Display)

**Abstract** : Modelling the hydrodynamics of charged colloids within ionic fluids is a challenging multi-physics problem. Rigid body particle motion is resisted by drag due to the viscosity of the fluid. Furthermore, ionic impurities give rise to electrical-double layers that can in turn induce flow of the solvent. In this paper, a moving mesh method for nano-rod electro-osmosis is introduced and applied to analyse particle trajectories in response to external electric fields.

## [00960] Hierarchical Low Rank Tensors and DNNs for High-dimensional Approximation

**Session Time & Room :**

00960 (1/3) : 3C (Aug.23, 13:20-15:00) @E506

00960 (2/3) : 3D (Aug.23, 15:30-17:10) @E506

00960 (3/3) : 3E (Aug.23, 17:40-19:20) @E506

**Type** : Proposal of Minisymposium

**Abstract** : The minisymposium aims at bridging the gap between low rank tensors and neural networks for learning of high-dimensional functions, in particular in the context of uncertainty quantification. The talks will highlight different aspects ranging from approximation to optimization.

The underlying motivation is to understand strengths and difficulties of network based representations and to identify structures and techniques that can be combined beneficially.

**Organizer(s)** : Martin Eigel, Lars Grasedyck

**Classification** : 65C40, 65N55, 65N30, 68T07

**Minisymposium Program :**

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00960 (1/3) : 3C @E506 [Chair: Lars Grasedyck]

## [04419] Low-rank tensor approximation of high-dimensional functions

**Format** : Talk at Waseda University

**Author(s)** : Helmut Harbrecht (University of Basel)Michael Griebel (University of Bonn)Reinhold Schneider (Technical University of Berlin)

**Abstract** : In this talk, we analyze tensor approximation schemes for high-dimensional functions in the continuous setting. To this end, we assume that the function to be approximated lies either in an isotropic Sobolev space or an anisotropic Sobolev space. We apply successively the truncated singular value decomposition in order to discuss the cost when approximating the function under consideration in the continuous analogues of tensor formats such as the Tucker tensor format or the tensor train format.

## [03995] Parameter-dependent multigrid method using low-rank tensor formats

**Format** : Talk at Waseda University

**Author(s)** : Tim Andreas Werthmann (RWTH Aachen University)Lars Grasedyck (RWTH Aachen University)

**Abstract** : We consider a parameter-dependent linear system motivated by a diffusion problem.

The combination of all finitely many parameters leads to an exponential scaling of the computational effort in the number of parameters, the so-called curse of dimensionality.

To break this curse, we use low-rank tensor formats to represent this system.

We introduce the parameter-dependent multigrid method to solve such a high-dimensional system within low-rank tensor formats.

## [04205] Alternating nonnegative factorizations for low-rank tensor formats

**Format** : Talk at Waseda University

**Author(s)** : Maren Klever (RWTH Aachen University)Lars Grasedyck (RWTH Aachen)Sebastian Kraemer (RWTH Aachen University)

**Abstract** : Low-rank tensor formats allow for efficient handling of high-dimensional objects.

If the quantity of interest is nonnegative, we want to preserve this property by constraining all cores to be nonnegative.

Common alternating strategies reduce the high-dimensional problem to a sequence of low-dimensional subproblems, but often suffer from slow convergence and persistence in local minima.

To reduce these inconveniences, we propose a new quasi-orthogonalization strategy as an intermediate step between the alternating minimization steps that preserves nonnegativity.

## [04392] Tensor surrogates for sensitivity analysis in the presence of polymorphic uncertainties

**Format** : Talk at Waseda University

**Author(s)** : Dieter Moser (RWTH Aachen University)

**Abstract** : Sensitivity analysis identifies the input parameters that have the greatest influence on model output. However, when input parameters are polymorphic, meaning that epistemic and aleatory uncertainty is present, traditional sensitivity analysis methods based on probabilistic modelling of the uncertainty have to be adapted.

A measurement of distances between polymorphic uncertainties is needed to measure the effect of the input parameters. In this talk, we will discuss how hierarchical tensor surrogates are beneficial for such an adapted sensitivity analysis.

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00960 (2/3) : 3D @E506 [Chair: Martin Eigel]

part\_2

## [02980] Weighted sparse and low-rank least squares approximation

**Format :** Talk at Waseda University

**Author(s) :** Philipp Trunschke (Nantes Université)Martin Eigel (WIAS Berlin)Anthony Nouy (Nantes Université)

**Abstract :** Many functions of interest exhibit weighted summability of their coefficients with respect to some dictionary of basis functions.

The resulting best  $n$ -term approximations can be estimated efficiently from samples.

We propose to encode the coefficients in a simultaneously sparse and low-rank tensor format to improve the efficiency of the algorithms performing this approximation.

Based on a weighted Stechkin lemma and the restricted isometry property, we provide approximation error and sample complexity bounds.

## [04007] Iteratively Reweighted Least Squares Recovery on Tensor Networks

**Format :** Talk at Waseda University

**Author(s) :** Sebastian Kraemer (RWTH Aachen University)

**Abstract :** A fundamental approach to tensor recovery traces back to affine rank minimization. We emphasize that the latter problem is always solved via asymptotic minimization of well-known log-det functions, in practice approachable through iteratively reweighted least squares. Additionally to local convergence properties, in numerical experiments, the theoretical phase transition for generic tensor recoverability becomes observable. Alternating optimization on tensor tree networks in turn allows to apply a relaxed method under minimal, polynomial complexity even in high dimensions.

## [04663] Empirical Tensor Train Approximation in Optimal Control

**Format :** Talk at Waseda University

**Author(s) :** Mathias Oster (TU Berlin)Reinhold Schneider (TU Berlin)

**Abstract :** We display two approaches to solve finite horizon optimal control problems. First we solve the Bellman equation numerically by employing the Policy Iteration algorithm. Second, we introduce a semiglobal optimal control problem and use open loop methods on a feedback level. To overcome computational infeasibility we use tensor trains and multi-polynomials, together with high-dimensional quadrature, e.g. Monte-Carlo. By controlling a destabilized version of viscous Burgers and a diffusion equation with unstable reaction term numerical evidence is given.

## [05144] Dynamical low-rank approximation of Vlasov-Poisson equations on polygonal spatial domains

**Format :** Talk at Waseda University

**Author(s) :** Andreas Zeiser (HTW Berlin)André Uschmajew (University of Augsburg)

**Abstract :** We consider dynamical low-rank approximation (DLRA) for the numerical simulation of Vlasov-Poisson equations based on separation of space and velocity variables, as proposed in several recent works. A less studied aspect is the incorporation of boundary conditions in the DLRA model. We use a variational formulation of the projector splitting which allows to handle inflow boundary conditions on piecewise polygonal spatial domains. Numerical experiments demonstrate the principle feasibility of this approach.

00960 (3/3) : 3E @E506 [Chair: Dieter Moser]

## [04645] Using Low-rank Tensor Formats in Neural Networks

**Format :** Talk at Waseda University

**Author(s) :** Thong Pham Hoang Le (RWTH Aachen University)Lars Grasedyck (RWTH Aachen)Janina Enrica Schütte (WIAS Berlin)Martin Eigel (WIAS Berlin)

**Abstract :** We investigate the use of low-rank tensor decompositions to improve the performance of neural network training. Specifically, we propose an approach that utilizes low-rank tensors to discretize the loss function of the neural network, which allows us to explore a larger parameter space than local methods such as Gradient Descent. Our approach could also facilitate improved weight initialization, further enhancing the network's performance.

## [03998] Adaptive Multilevel Neural Networks for parametric PDEs with Error Estimation

**Format :** Talk at Waseda University

**Author(s) :** Janina Enrica Schütte (WIAS Berlin)Martin Eigel (WIAS)

**Abstract :** We focus on efficiently solving high dimensional, parameter-dependent partial differential equations. To approximate the parameter-to-solution map, different model classes have been considered, including low-rank tensor representations and neural network architectures.

In our work, a new multilevel neural network architecture is combined with an adaptive scheme including a solver based on a multilevel decomposition, classical reliable finite element error estimators, and a refinement strategy for the considered finite element grids. We show expressivity results and numerical experiments for the derived networks.

## [00961] Reinforcement Learning for Financial Modeling

**Session Time & Room :** 4C (Aug.24, 13:20-15:00) @A208

**Type :** Proposal of Minisymposium

**Abstract :** This minisymposium, sponsored by the SIAM activity group in Financial Mathematics, focuses on the development of novel reinforcement learning paradigms for solving problems in financial mathematics. The RL paradigm aims to approximate solutions to stochastic control problems in discrete time in a manner that is agnostic to the dynamics of environment and its response to agents' actions. The collection of talks covers the incorporation of time-consistent risk-measures into RL, provides explicit error bounds on exploratory control, and develops a new approach to eliciting agents' risk preferences in an novel inverse RL framework.

**Organizer(s) :** Sebastian Jaimungal  
**Sponsor :** This session is sponsored by the SIAM Activity Group on Financial Mathematics and Engineering.

**Classification :** 93E20, 91G80, 49N45

**Minisymposium Program :**

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00961 (1/1) : 4C @A208 [Chair: Sebastian Jaimungal]

## [03063] Reinforcement learning for mean field games and mean field control problems, with applications to finance

**Format :** Talk at Waseda University

**Author(s) :** Mathieu Lauriere (NYU Shanghai)

**Abstract :** Mean field games have been introduced to study Nash equilibria in large populations of strategic agents, while mean field control problems aim at modeling social optima in large groups of cooperative agents. These frameworks have found a wide range of applications, from economics and finance to social sciences and biology. In the past few years, the question of learning equilibria and social optima in a mean field setting has attracted a growing interest. In this talk, I will discuss several model-free methods based on reinforcement learning. Numerical experiments on stylized examples of financial models will be presented.

## [03255] Learning Risk Aversion with Inverse Reinforcement Learning via Interactive Questioning

**Format :** Talk at Waseda University

**Author(s) :** Ziteng Cheng (University of Toronto)Anthony Coache (University of Toronto)Sebastian Jaimungal (University of Toronto)

**Abstract :** This paper proposes a novel framework for identifying an agent's risk aversion using interactive questioning. We assume that the agent's risk aversion is characterized by a spectral risk measure chosen from a finite set of candidates. We show that asking the agent to choose from a finite set of random costs, which may depend on their previous answers, is an effective means of identifying the agent's risk aversion. Specifically, we prove that the agent's risk aversion can be identified as the number of questions tends to infinity, and the questions are randomly designed. We also develop an algorithm for designing optimal questions and provide empirical evidence that our method learns risk aversion significantly faster than randomly designed questions in a simulated

environment. Our framework has important applications in robo-advising and provides a new approach for identifying an agent's risk preferences.

### [04804] Fisher-Rao Gradient Descent for Stochastic Control Problems.

**Format :** Talk at Waseda University

**Author(s) :** Lukasz Szpruch (University of Edinburgh/The Alan Turing Institute )David Siska (University of Edinburgh )Bekzhan Kerimkulov (University of Edinburgh )

**Abstract :** We study the convergence of Gradient and Mirror Descent schemes for approximating solutions to stochastic control problems with measure-valued controls in continuous time. By exploiting Pontryagin Optimality Principle, these rely on solving forward and backward (adjoint) equations and performing static optimisation problems regularised with Bregman divergence and can be interpreted as implicit and explicit discretisations of Fisher-Rao gradient flow. In the general (non-convex) case, we show that the objective function decreases along the gradient step. Moreover, in the (strongly) convex case, when Pontryagin Optimality Principle provides a sufficient condition for optimality, we prove that the objective converges at the (exponential) linear rate to its optimal value. The main technical difficulty is to show that stochastic control problem admits suitable relative smoothness and convexity properties. These are obtained by utilising the theory of Bounded Mean Oscillation (BMO) martingales required for estimates on the adjoint Backward Stochastic Differential Equation (BSDE).

### [05398] Risk Budgeting Allocation for Dynamic Risk Measures

**Format :** Talk at Waseda University

**Author(s) :** Sebastian Jaimungal (University of Toronto)Silvana Manuela Pesenti (University of Toronto)Yuri Saporito (FGV)Rodrigo Targino (FGV)

**Abstract :** We develop an approach for risk budgeting allocation -- a risk diversification portfolio strategy -- where risk is measured using time-consistent dynamic risk measures. For this, we introduce a notion of dynamic risk contributions that generalise the classical Euler contributions and which allow us to obtain dynamic risk contributions in a recursive manner. Moreover, we prove that, for the class of dynamic coherent distortion risk measures, the risk allocation problem may be recast as a sequence of convex optimisation problems and, leveraging the elicitability of dynamic risk measures, develop an actor-critic approach to solve for risk budgeting strategy using deep learning.

## [00963] Nonconvex and nonsmooth optimization

**Session Time & Room :** 5B (Aug.25, 10:40-12:20) @A206

**Type :** Proposal of Minisymposium

**Abstract :** Optimization is a powerful tool to harnesses the power of big data in statistics, machine learning, compressed sensing, etc. Many modern optimization problems involve nonconvexity and nonsmoothness which creates a major gap between the actual solutions being computed and the global optimizers that traditional analysis investigates. Such challenges are new opportunities for researchers to make fundamental contributions to analytical and numerical methods for optimization. This mini-symposium aims to gather researchers with similar interests in optimization and foster in-depth discussions.

**Organizer(s) :** Sunyoung Shin

**Classification :** 90C26, 65K05

**Minisymposium Program :**

00963 (1/1) : 5B @A206 [Chair: Sunyoung Shin]

### [01977] A lifted L1 framework for sparse recovery

**Format :** Talk at Waseda University

**Author(s) :** Yifei Lou (University of Texas at Dallas)Yaghoub Rahimi (Georgia Institute of Technology)Sung Ha Kang (Georgia Institute of Technology)

**Abstract :** Motivated by re-weighted  $\ell_1$  approaches for sparse recovery, we propose a lifted  $\ell_1$  (LL1) regularization that can be generalized to several popular regularizations in the literature. During the course of reformulating the existing methods into our framework, we discover two types of lifting functions that can guarantee that the

proposed approach is equivalent to the  $\ell_0$  minimization. Computationally, we design an efficient algorithm via the alternating direction method of multiplier (ADMM) and establish the convergence for an unconstrained formulation. Experimental results are presented to demonstrate how this generalization improves sparse recovery over the state-of-the-art.

### [02344] A generalized formulation for group selection via ADMM

**Format :** Talk at Waseda University

**Author(s) :** Sunyoung Shin (Pohang University of Science and Technology)Chengyu Ke (Southern Methodist University)Yifei Lou (University of Texas at Dallas)Miju Ahn (Southern Methodist University)

**Abstract :** The talk considers a statistical learning model where the model coefficients have a pre-determined group sparsity structure. A loss function is combined with a regularizer to recover the sparsity. We analyze the stationary solution of the formulation, obtaining a sufficient condition for the stationary solution to achieve optimality. We develop an efficient ADMM algorithm, showing the iterates converge to a stationary solution under certain conditions. With the algorithm implemented for GLM, we perform numerical experiments.

### [02395] A novel tensor regularization of nuclear over Frobenius norms for low rank tensor recovery

**Format :** Talk at Waseda University

**Author(s) :** Huiwen Zheng (Southern University of Science and Technology)Yifei Lou (University of Texas at Dallas)Guoliang Tian (Southern University of Science and Technology)Chao Wang (Southern University of Science and Technology)

**Abstract :** In this talk, we consider low-rank tensor recovery (LRTR) problems, which include the low-rank tensor completion (LRTC) problem and the tensor robust principal component analysis (TRPCA) problem. Based on tensor singular value decomposition (t-SVD), we use the ratio of the tensor nuclear norm and tensor Frobenius norm as a new nonconvex surrogate of tensor rank in our models. We adopt the alternating direction method of multipliers (ADMM) to tackle the model and analyze the convergence of the models. Extensive experiments demonstrate the superiority of the proposed models.

### [02672] Tractable continuous approximations for a constraint selection problem

**Format :** Online Talk on Zoom

**Author(s) :** Miju Ahn (Southern Methodist University)Harsha Gangammanavar (Southern Methodist University)David Troxell (Stanford University)

**Abstract :** This presentation introduces a constraint selection problem where the decision-maker solves an optimization problem with a set of constraints that are preferred to be satisfied. We formulate the problem as a cardinality minimization problem (CMP) that penalizes the number of unsatisfied such soft constraints using an indicator function. Our approach reformulates the discrete CMP as continuous problems. We present an equivalent formulation of a mathematical program with complementarity constraints and an approximation as a difference-of-convex program. The stationary solutions of the alternative formulations are investigated, emphasizing the recovery of the local solutions of the CMP. Our numerical study results demonstrate our method's effectiveness in enforcing desired conditions on several applications.

## [00965] New mathematical trends in weather prediction and inverse problems

**Session Time & Room :**

00965 (1/2) : 5C (Aug.25, 13:20-15:00) @F309

00965 (2/2) : 5D (Aug.25, 15:30-17:10) @F309

**Type :** Proposal of Minisymposium

**Abstract :** In applied mathematics including inverse problems, problems are often ill-posed and/or data are limited. Such difficulties have been treated in different subfields of science: medical imaging, data assimilation in numerical weather prediction, etc. In this minisymposium, researchers from data assimilation and inverse problems will gather and discuss different tools and ideas in applied mathematics to handle complicated problems

and incomplete data.

**Organizer(s)** : Shunji Kotsuki, Wei Li, Manabu Machida

**Classification** : 37Nxx, 65Mxx, 65Nxx, 65Pxx

**Minisymposium Program :**

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00965 (1/2) : 5C @F309

## [03741] Gaussian Assimilation of non-Gaussian Image Data via Pre-Processing by Variational Auto-Encoder (VAE)

**Author(s)** : Daisuke Hotta (Meteorological Research Institute, Japan Meteorological Agency)

**Abstract** : Assimilation of image data such as satellite images with conventional data assimilation methods is challenging due to non-Gaussian error distribution, dimensional redundancy, and strong inter-pixel correlations. While several techniques have been proposed to address each of these issues, no single method can simultaneously handle them all. Here we propose to use a Variational AutoEncoder to resolve all three difficulties. A preliminary assessment with a toy model shows promising results.

## [04216] Implementing local ensemble transform Kalman filter to reservoir computing for improving weather forecast

**Author(s)** : Mao Ouyang (Chiba University)Shunji Kotsuki (Chiba University)

**Abstract** : Data assimilation (DA) improves the numerical weather prediction (NWP) by combining the model forecast and observational data. The forecasts were usually obtained from a physical-based model, but recent studies reported that the reservoir computing (RC) could be implemented to surrogate both the small- and intermediate-scale physical models. This study implemented the DA, i.e., local ensemble transform Kalman filter, in both the physic-based and RC-surrogated models and compared their performances in the improvement of forecasts.

## [04315] Sparse optimization of inverse problems regularized with infimal-convolution-type functionals

**Author(s)** : Marcello Carioni (University of Twente)

**Abstract** : The infimal convolution of functionals is a convex-preserving operation that have been used to construct regularizers for inverse problems by optimally combining features of two or more functionals. In this talk, we analyze the infimal convolution regularization from a sparse optimization point of view. First, we discuss optimal transport-type energies. Then, we consider the infimal convolution of a parametrized family of functionals and we develop optimization methods taking advantage of the sparsity in the parameters.

## [04562] Efficient data-driven regularization for ill-posed inverse problems in imaging

**Author(s)** : Subhadip Mukherjee (University of Bath, UK)Marcello Carioni (University of Twente)Ozan Öktem (KTH Royal Institute of Technology)Carola-Bibiane Schönlieb (University of Cambridge)

**Abstract** : In recent years, data-driven regularization has led to impressive performance for image reconstruction problems in various scientific applications, e.g., medical imaging. We propose a new adversarial learning approach for imaging inverse problems by combining an iteratively unrolled network with a deep regularizer using ideas from optimal transport. The resulting unrolled adversarial regularization approach is shown to be provably stable, efficient in terms of image reconstruction time, and competitive with supervised methods in empirical performance.

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00965 (2/2) : 5D @F309

## [05386] Inverse problems for nonlocal PDEs with applications to quantum optics

**Author(s)** : John Schotland (Yale University)

**Abstract** : I will discuss recent work with Jeremy Hoskins and Howard Levinson on reconstruction methods for inverse problems for nonlocal PDEs. Applications to quantum optics will be discussed.

## [05472] Implicit Ensemble Tangent Linear Models (IETLMs) for model differentiation

**Author(s)** : Craig H Bishop (University of Melbourne)Nathan W Eizenberg (University of Melbourne)

**Abstract** : Ideally, Tangent Linear Models (TLMs) predict the difference between perturbed and unperturbed non-linear forecasts of interest. The adjoint of a TLM gives the gradient of the non-linear model and is used in 4DVar data assimilation and in adjoint-based Forecast Sensitivity to Observation Impact (FSOI). The Local Ensemble Tangent Linear Model's (LETLM) accuracy has been shown to be limited by its inability to account for implicit time stepping. Here we derive Implicit Ensemble TLMs (IETLMs) that, at most, require the number of independent ensemble members to be equal to the number of variables in the implicit computational stencil. The accuracy of the IETLM in the linear regime is confirmed using an implicitly time stepped Lorenz 96 model and a 9-member ensemble. IETLMs feature two sparse matrices: matrix N that operates on an initially unknown future time perturbation, and matrix L that operates on the current time perturbation. For ensemble perturbations in the non-linear regime, we develop a Diagonally Robust (DR) IETLM that reduces the chances of N becoming ill-conditioned. The performance of the DR IETLM was compared with traditional TLM performance using IETLM ensemble perturbations whose "Gilmour et al., 2001" measure of non-linearity ranged up to the non-linearity of operational 32 hr ensemble forecast perturbations. Over a wide range of non-linearity, the DR IETLM performance was found to match that of the traditional TLM provided the initial standard deviation of the ensemble perturbations was  $\sqrt{2}$  times the standard deviation of the test perturbations. Ideal FSOI requires the adjoint of a TLM that accurately predicts the known difference between corrected and uncorrected non-linear forecasts. The DR IETLM was found to meet this FSOI accuracy requirement much more closely than the traditional TLM when the ensemble perturbations were created by subtracting the corrected forecast from ensemble members that were centred on the uncorrected forecast. Finally, if time permits, a method for reducing the size of the ensemble required to produce accurate TLMs will be described.

## [05482] Advances in Integrating AI and Machine Learning with Data Assimilation for Weather Prediction

**Author(s)** : Stephen G Penny (Sofar Ocean)

**Abstract** : Capabilities of AI/ML methods necessary for online data assimilation (DA), such as accounting for accurate model response to perturbations in initial conditions, will be discussed in the context of a variety of increasing complexity dynamical systems ranging from Lorenz-96, to quasi-geostrophic (QG) dynamics, to surface QG turbulence. In this context, the success of recurrent neural networks for achieving this goal will be demonstrated by integrating with conventional DA methods such as the Ensemble Kalman Filter (EnKF) and 4D-Var. Dynamical invariants such as the Lyapunov spectrum will also be explored both as a useful diagnostic and as tool to accelerate the training of ML models. Caveats regarding training on simulated datasets and reanalysis datasets will also be discussed.

## [05497] Learned weakly convex regularisers in inverse problems

**Author(s)** : Zakhar Shumaylov (University of Cambridge)Jeremy Budd (University of Bonn)Carola-Bibiane Schönlieb (University of Cambridge)

**Abstract** : In this talk, we consider the problem of learned regularisation in the area of imaging inverse problems. By showing limitations of existing methods arising in adversarial regularisation, we propose usage of weakly convex regularisers to address the problems. We provide a construction of weakly convex input neural networks and discuss convergence guarantees for the variational problem. We provide numerical evidence to exemplify their usage in the settings of sparse and limited angle computed tomography reconstruction.

## [00966] Theoretical and computational advances in measure transport

**Session Time & Room :**

00966 (1/3) : 1C (Aug.21, 13:20-15:00) @F411

00966 (2/3) : 1D (Aug.21, 15:30-17:10) @F411

00966 (3/3) : 1E (Aug.21, 17:40-19:20) @F411

**Type :** Proposal of Minisymposium

**Abstract :** Transportation of measures is an important topic in applied mathematics based on constructing invertible transformations between random variables. These transformations can include deterministic maps, plans and stochastic processes. In recent years, this broad topic has seen wide applications for generative modeling, inference, and comparing probability distributions. Despite these successes, efficiently constructing these transformations remains challenging, especially in high-dimensional problems with complex data manifolds. This minisymposium will present novel statistical analysis and computational methods that widen the breadth of transport methods in statistics and scientific computing applications.

**Organizer(s) :** Ricardo Baptista, Arnaud Doucet, Tiangang Cui, Youssef Marzouk

**Classification :** 49Q22, 65C20

**Minisymposium Program :**

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00966 (1/3) : 1C @F411 [Chair: Ricardo Baptista]

## [05226] Optimal transport map estimation in general function spaces

**Format :** Talk at Waseda University

**Author(s) :** Vincent Divol (Université PSL)Jonathan Niles-Weed (New York University)Aram Pooladian (New York University)

**Abstract :** We consider the problem of estimating the optimal transport map between a (fixed) source distribution  $P$  and an unknown target distribution  $Q$ , based on samples from  $Q$ . The estimation of such optimal transport maps has become increasingly relevant in modern statistical applications, such as generative modeling. At present, estimation rates are only known in a few settings (e.g. when  $P$  and  $Q$  have densities bounded above and below and when the transport map lies in a Hölder class), which are often not reflected in practice. We present a unified methodology for obtaining rates of estimation of optimal transport maps in general function spaces. Our assumptions are significantly weaker than those appearing in the literature: we require only that the source measure  $P$  satisfies a Poincaré inequality and that the optimal map be the gradient of a smooth convex function that lies in a space whose metric entropy can be controlled. As a special case, we recover known estimation rates for bounded densities and Hölder transport maps, but also obtain nearly sharp results in many settings not covered by prior work. For example, we provide the first statistical rates of estimation when  $P$  is the normal distribution and the transport map is given by an infinite-width shallow neural network.

## [04080] TBA

**Author(s) :** Augusto Gerolin (Canada Research Chair and University of Ottawa)

**Abstract :** TBA

## [04165] Efficient subspace modeling via transport transforms

**Format :** Talk at Waseda University

**Author(s) :** Shiyiing Li (University of North Carolina - Chapel Hill)Gustavo Rohde (University of Virginia)Akram Aldroubi (Vanderbilt University)Abu Hasnat Rubaiyat (University of Virginia)Yan Zhuang (NIH)Mohammad Shifat-E-Rabbi (University of Virginia)Xuwang Yin (Center for AI Safety )

**Abstract :** When data is generated through deformations of certain template distributions, transport-based transforms often linearize data clusters which are nonlinear in the original domain. We will describe convexification properties of several transport transforms under various generative modeling assumptions, enabling efficient modeling of data classes as subspaces in the transform domain. Such subspace representations also give rise to accurate machine learning algorithms with low computational cost. We will show applications for image and signal classification.

## [04063] Conditional simulation through the data-driven optimal transport barycenter problem

**Format :** Talk at Waseda University

**Author(s) :** Esteban Gregorio Tabak (New York University, Courant Institute)

**Abstract :** A methodology is proposed to generate samples from a conditional probability distribution, with factors that are either known explicitly, up to discovery or only by association. The procedure pushes forward the conditional distribution to its barycenter through particle flows, whose inverse provides the simulation sought. Idiosyncratic factors are included through subsampling. The methodology serves as a conditional generator, to eliminate batch effects, to uncover hidden factors and to predict and optimize trajectories under treatment.

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00966 (2/3) : 1D @F411 [Chair: Tiangang Cui]

## [04311] On the Monge gap and the MBO feature-sparse transport estimator.

**Format :** Talk at Waseda University

**Author(s) :** marco cuturi (Apple)

**Abstract :** This talk will cover two recent works aimed at estimating Monge maps from samples. In the first part (in collaboration with Théo Uscidda) I will present a novel approach to train neural networks so that they mimic Monge maps for the squared-Euclidean cost. In that field, a popular approach has been to parameterize dual potentials using input convex neural networks, and estimate their parameters using SGD and a convex conjugate approximation. We present in this work a regularizer for that task that is conceptually simpler (as it does not require any assumption on the architecture) and which extends to non-Euclidean costs. In the second part (in collaboration with Michal Klein and Pierre Ablin), I will show that when adding to the squared-Euclidean distance an extra translation-invariant cost, the Brenier theorem translates into the application of the proximal mapping of that extra term to the derivative of the dual potential. Using an entropic map to parameterize that potential, we obtain the Monge-Bregman-Occam (MBO) estimator, which has the defining property that its displacement vectors  $T(x) - x$  are sparse, resulting in interpretable OT maps in high dimensions.

## [05300] Simulation-Free Generative Modeling with Neural ODEs

**Format :** Talk at Waseda University

**Author(s) :** Ricky Tian Qi Chen (Meta AI)

**Abstract :** Standard diffusion models offer a simulation-free method of training continuous-time transport maps but are typically restricted to linear stochastic processes. In this talk, I will discuss Flow Matching, a training objective that allows regressing onto the generating vector field instead of the score vector field. This allows more flexibility in the design of probability paths, extends seamlessly to general manifolds, and brings the model closer to optimal transport solutions.

## [04077] Diffusion Schrödinger Bridge Matching

**Format :** Talk at Waseda University

**Author(s) :** Yuyang Shi (Oxford university) Valentin De Bortoli (ENS Ulm) Andrew Campbell (Oxford University) Arnaud Doucet (Oxford University)

**Abstract :** Solving transport problems, i.e. finding a map transporting one given distribution to another, has numerous applications in machine learning. Novel mass transport methods motivated by generative modeling have recently been proposed, e.g. Denoising Diffusion Models (DDMs) and Flow Matching Models (FMMs) implement such a transport through a Stochastic Differential Equation (SDE) or an Ordinary Differential Equation (ODE). However, while it is desirable in many applications to approximate the deterministic dynamic Optimal Transport (OT) map which admits attractive properties, DDMs and FMMs are not guaranteed to provide transports close to the OT map. In contrast, Schrödinger bridges (SBs) compute stochastic dynamic mappings which recover entropy-regularized versions of OT. Unfortunately, existing numerical methods approximating SBs either scale poorly with dimension or accumulate errors across iterations. In this work, we introduce Iterative Markovian Fitting, a new methodology for solving SB problems, and Diffusion Schrödinger Bridge Matching (DSBM), a novel numerical algorithm for computing IMF iterates. DSBM significantly improves over previous SB numerics and recovers as special/limiting cases various recent transport methods. We demonstrate the performance of DSBM on a variety of problems.

## [05473] Diffusion Bridge Mixture Transports, Schrödinger Bridge Problems and Generative Modeling

**Format :** Talk at Waseda University

**Author(s) :** Stefano Peluchetti (Cogent Labs)

**Abstract :** The dynamic Schrödinger bridge problem seeks a stochastic process that defines a transport between two target probability measures, while optimally satisfying the criteria of being closest, in terms of Kullback-Leibler divergence, to a reference process.

We propose a novel sampling-based iterative algorithm, the iterated diffusion bridge mixture (IDBM) procedure, aimed at solving the dynamic Schrödinger bridge problem.

The IDBM procedure exhibits the attractive property of realizing a valid transport between the target probability measures at each iteration.

We perform an initial theoretical investigation of the IDBM procedure, and carry out numerical experiments illustrating the competitive performance of the IDBM procedure.

Recent advancements in generative modeling employ the time-reversal of a diffusion process to define a generative process that approximately transports a simple distribution to the data distribution.

As an alternative, we propose utilizing the first iteration of the IDBM procedure as an approximation-free method for realizing this transport.

This approach offers greater flexibility in selecting the generative process dynamics and exhibits accelerated training and superior sample quality over larger discretization intervals.

00966 (3/3) : 1E @F411 [Chair: Youssef Marzouk]

## [05484] Neural Optimal Transport for Single-Cell Biology

**Format :** Online Talk on Zoom

**Author(s) :** Charlotte Bunne (ETH Zurich)

**Abstract :** To accurately predict the responses of a patient's tumor cells to a cancer drug, it is vital to recover the underlying population dynamics and fate decisions of single cells. However, measuring molecular properties of single cells requires destroying them. As a result, a cell population can only be monitored with sequential snapshots, obtained by sampling a few particles that are sacrificed in exchange for measurements. In order to reconstruct individual cell fate trajectories, as well as the overall dynamics, one needs to re-align these unpaired snapshots, in order to guess for each cell what it might have become at the next step. Optimal transport theory can provide such maps, and reconstruct these incremental changes in cell states over time. This celebrated theory provides the mathematical link that unifies the several contributions to model cellular dynamics that we present here: Inference from data of an energy potential best able to describe the evolution of differentiation processes (Bunne et al., 2022), building on the Jordan-Kinderlehrer-Otto (JKO) flow; recovery of differential equations modeling the stochastic transitions between cell fates in developmental processes (Bunne et al., 2023) through Schrödinger bridges; as well as zero-sum game theory models parameterizing distribution shifts upon interventions, which we employ to model heterogeneous responses of tumor cells to cancer drugs (Bunne et al., 2022, 2023).

## [04231] Tensor-train methods for sequential state and parameter learning in state-space models

**Format :** Talk at Waseda University

**Author(s) :** Tiangang Cui (Monash University)Yiran Zhao (Monash University)

**Abstract :** We consider sequential state and parameter learning in state-space models with intractable state transition and observation processes. By exploiting low-rank tensor-train (TT) decompositions, we propose new sequential learning methods for joint parameter and state estimation under the Bayesian framework. Our key innovation is the introduction of scalable function approximation tools such as TT for recursively learning the sequentially updated posterior distributions. The function approximation perspective of our methods offers tractable error analysis and potentially alleviates the particle degeneracy faced by many particle-based methods. In addition to the new insights into algorithmic design, our methods complement conventional particle-based methods. Our TT-based approximations naturally define conditional Knothe-Rosenblatt (KR) rearrangements that lead to filtering, smoothing, and path estimation accompanying our sequential learning algorithms, which open the door to removing potential approximation bias. We also explore several preconditioning techniques based on either linear or nonlinear KR rearrangements to enhance the approximation power of TT for practical problems. We demonstrate the efficacy and efficiency of our proposed methods on several state-space models, in which our methods achieve state-of-the-art estimation accuracy and computational performance.

## [04473] Tensor train approximation of deep transport maps for Bayesian inverse problems.

**Format :** Talk at Waseda University

**Author(s) :** Tiangang Cui (Monash University)Sergey Dolgov (University of Bath)Robert Scheichl (Heidelberg University)Olivier Zahm (Universite Grenoble Alpes, Inria)

**Abstract :** We develop a deep transport map for sampling concentrated distributions defined by an unnormalised density function. We approximate the target distribution as the pushforward of a reference distribution under a composition of transport maps formed by tensor-train approximations of bridging densities. We propose two bridging strategies: tempering the target density, and smoothing of an indicator function with a sigmoids. The latter opens the door to efficient computation of rare event probabilities in Bayesian inference problems.

## [05065] Accelerated Interacting Particle Transport for Bayesian Inversion

**Format :** Talk at Waseda University

**Author(s) :** Martin Eigel (WIAS) Robert Gruhlke (FU Berlin) David Sommer (WIAS)

**Abstract :** Ensemble methods have become ubiquitous for solving Bayesian inference problems. State-of-the-art Langevin samplers such as the Ensemble Kalman Sampler (EKS) and Affine Invariant Langevin Dynamics (ALDI) rely on many evaluations of the forward model, which we try to improve. First, adaptive ensemble enrichment strategies are discussed. Second, analytical consistency guarantees of the ensemble enrichment for linear forward models are presented. Third, a homotopy formalism for involved distributions is introduced.

## [00967] Stochastic Dynamical Systems and Applications in Data Science

**Session Time & Room :**

00967 (1/3) : 1D (Aug.21, 15:30-17:10) @E502

00967 (2/3) : 1E (Aug.21, 17:40-19:20) @E502

00967 (3/3) : 2C (Aug.22, 13:20-15:00) @E502

**Type :** Proposal of Minisymposium

**Abstract :** The theory of Dynamical Systems has helped us to analyze models in various quantitative and qualitative ways, but when considering noisy data with tools in stochastic analysis, there are still challenges in many applications to get precise models for different kinds of processes. On the other hand, lots of innovative methods in data science are now opening up new research directions and broadening the range of research fields where conventional dynamical systems can play a role. Therefore, it is important to consider interplanetary research fields between stochastic dynamics and machine learning: how to analyze stochastic dynamic systems based on observation data instead of studying models analytically? And how to analyze Machine Learning algorithms using tools from the theory of stochastic dynamical systems? In this minisymposium, we seek to find a deeper understanding of the mathematical foundations of the state-of-the-art ideas and techniques in data science as well as its applications in understanding stochastic dynamics, through algorithm development, theoretical analysis, and/or computational implementation. Fields can be covered by but are not limited to Stochastic Analysis, Inverse Problems, Stochastic Optimal Control, Numerical Analysis, Optimization, Topological Data Analysis, Nonparametric Statistics, Uncertainty Quantification, Meta Learning and Deep Reinforcement Learning, etc.

**Organizer(s) :** Ting Gao, Xiaoli Chen, Jinqiao Duan

**Classification :** 60H10, 62M20, 93E10, 65Z05, 82C05

**Minisymposium Program :**

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00967 (1/3) : 1D @E502

## [02120] Föllmer flows: contraction, sampling and generative learning

**Author(s) :** Ting Gao (Huazhong University of Science and Technology) Yuling Jiao (Wuhan University)

**Abstract :** We construct a unit-time flow on the Euclidean space, termed the Föllmer flow, whose flow map at time 1 pushes forward a standard Gaussian measure onto a general target measure. We study the well-posedness of the Föllmer flow and establish the Lipschitz property of the flow map at time 1. We apply the Lipschitz mapping to several rich classes of probability measures on deriving functional inequalities with dimension-free constants, sampling and generative learning.

## [02122] Stochastic systems via rough path theory: theory and numerics

**Author(s) :** Ting Gao (Huazhong University of Science and Technology) Hoang Duc Luu (MPI MIS & IMH-VAST)

**Abstract :** This talk presents stochastic differential equations driven by Hölder noises, which can be solved in the pathwise sense using rough path theory. The asymptotic dynamics of the system can be studied under random dynamical systems, and results on existence of random pullback attractors can be derived for dissipative systems. The numerical attractor of the discrete system is proved to converge to the one of the continuous system as the time step tends to zero.

## [02124] Data-driven method to learn polymer dynamics

**Author(s)** : Xiaoli Chen (National University of Singapore)

**Abstract** : We propose a machine learning approach where we construct reduced thermodynamic coordinates and interpret the dynamics of these coordinates directly from microscopic stochastic trajectory data. Our approach allows the creation of custom thermodynamics that elucidates macroscopic dynamical landscapes and facilitates subsequent analysis and control. We demonstrate our method on a long polymer chain in an externally applied field by showing that only three learnt thermodynamic coordinates are sufficient to build a dynamical landscape of unfolding.

## [02123] Transition Phenomena in Non-Gaussian Stochastic Dynamical Systems

**Author(s)** : Ting Gao (Huazhong University of Science and Technology)Jinqiao Duan (Illinois Institute of Technology and Great Bay University )

**Abstract** : Dynamical systems under non-Gaussian Levy fluctuations manifest as nonlocality at a certain “macroscopic” level. Transition phenomena are special events for evolution from one metastable state to another. Examples for such events are phase transition, pattern change, gene transcription, climate change, abrupt shifts, extreme transition, and other rare events. The most probable transition pathways are the maximal likely trajectory (in the sense of optimizing a probability or an action functional) between metastable states.

00967 (2/3) : 1E @E502

## [02126] Understanding the diffusion models by conditional expectations

**Author(s)** : Ting Gao (Huazhong University of Science and Technology)Yubin Lu (Illinois Institute of Technology)

**Abstract** : We provide several mathematical analyses of the diffusion model in machine learning. The drift term of the backwards sampling process is represented as a conditional expectation involving the data distribution and the forward diffusion. The training process aims to find such a drift function by minimizing the mean-squared residue related to the conditional expectation. We derive a new target function and associated loss and illustrate the theoretical findings with several numerical examples.

## [02127] Early-warning indicator of transition time for noise-induced critical transition of Atlantic Meridional Overturning Circulation

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**Author(s)** : Ting Gao (Huazhong University of Science and Technology)Yayun Zheng (Jiangsu University)

**Abstract** : We develop an effective and general early-warning indicator for critical transition. The indicator of most probable transition time based on the critical tube is proposed by Onsager-Machlup method based on a critical tube probability. The approach is applied to investigate the abrupt transition from the strong to the weak mode in a thermohaline circulation model. The indicator of the most probable transition time can provide important insights for predicting future abrupt climate transitions.

## [02128] Solving the Non-local Fokker-Planck Equations by Physics-informed Neural Networks

**Author(s)** : Ting Gao (Huazhong University of Science and Technology)Senbao Jiang (Illinois Institute of Technology)Xiaofan Li (Illinois Institute of Technology)

**Abstract** : We present trapz-PiNNs, incorporated with a modified trapezoidal rule recently developed for accurately evaluating fractional Laplacian and solve the space-fractional Fokker-Planck equations in 2D/3D. We demonstrate trapz-PiNNs have high expressive power through predicting solution with low  $L^2$  relative error by a variety of numerical examples. The trapz-PiNN is able to solve PDEs with fractional Laplacian with arbitrary  $0 < \alpha < (0, 2)$  and on rectangular domains. It could be generalized into higher dimensions or other bounded domains.

## [02129] Emergent Short-range Memory in Stochastic Gradient Noise and Its Implications on Generalization

**Author(s)** : Ting Gao (Huazhong University of Science and Technology)Jiangshe Zhang (Xi'an Jiaotong University)

**Abstract** : Investigating stochastic gradient descent (SGD) from the perspective of stochastic differential equations (SDEs) is quite popular in the deep learning community. In this talk, I will present an analytical result on modeling SGD with SDEs driven by fractional Brownian motion, which reveals the escaping efficiency when trapped in local minima. From the optimization point of view, I will further show how we can relate the smoothness of the optimization pathway to the generalization ability.

00967 (3/3) : 2C @E502

## [03377] Modeling and learning methods applied to collective motion in biology

**Author(s)** : James Greene (Clarkson University)Ming Zhong (Illinois Institute of Technology)

**Abstract** : From groups of cells to groups of humans, collective motion is ubiquitous in biological systems . Inspired by phototaxis, we develop minimal mathematical models that exhibit the emergence of social structure in Cucker-Smale type pairwise interaction models. Numerical and analytical results are provided, which show the emergence of linear spatial structures. We also present methods by which local interaction rules may be learned from trajectory data, and apply these techniques to cancer migration models.

## [03399] Neural architectures for identifying stochastic differential equations

**Author(s)** : Ali Hasan (Duke University)Joao Pereira (Instituto Nacional de Matemática Pura e Aplicada)Haoming Yang (Duke University)Sina Farsiu (Duke University)Vahid Tarokh (Duke University)

**Abstract** : In this work, we will describe a variational framework to recover the parameters of a latent stochastic differential equation (SDE) from high dimensional observations. We prove that, in the limit of infinite data, the true parameters can be recovered up to an isometry and numerically illustrate the efficacy of the method. We finally discuss connections to McKean-Vlasov SDEs when using neural network parameterizations of SDEs and present numerical examples in machine learning applications.

## [03687] Deep learning framework for solving Fokker-Planck equations with low-rank separation representation

**Author(s)** : Yong Xu (Northwestern polytechnical university)

**Abstract** : An insightful deep learning framework is proposed in this study for solving the well-known Fokker-Planck (FP) equations that quantify the evolution of the probability density function. It efficiently reduces the demand of training data in acquiring precise integrations of special normalizing conditions when using neural network (NN). While it also avoids the exponential increase in training data as dimension increases. Instead of all hypercubic discrete points, the inputs of each NN only require one-dimensional discrete data. Without loss of generality, to solve a d-dimensional FP equation, d NNs are employed and assembled into a low-rank separation representation. The FP, boundary, and integral operators are then re-expressed in separation representation. It enables the constructed loss function performs simple vector operations, because the complicated d-dimensional operators are replaced by a set of onedimensional operators. A tractable strategy is presented for the selection of separation rank inspired by the system's potential function, although selecting an appropriate separation rank is still an open issue. Typical numerical examples reveal that the proposed algorithm is effective and superior for solving the FP equations. The suggested framework is applicable and has considerable potential in various areas of engineering and applied sciences.

# [00969] Eigenvalue Problems in Electronic Structure Calculations

**Session Time & Room :**

00969 (1/3) : 4C (Aug.24, 13:20-15:00) @G709

00969 (2/3) : 4D (Aug.24, 15:30-17:10) @G709

00969 (3/3) : 4E (Aug.24, 17:40-19:20) @G709

**Type :** Proposal of Minisymposium

**Abstract :** The first principles electronic structure calculations have become important tools for studying the material mechanism, understanding and predicting the material properties, and have achieved great success. The key mathematical models for electronic structure calculations are eigenvalue problems or equivalent forms. There are still many challenges on the design of highly efficient and highly accurate computational methods for dealing these eigenvalue problems or equivalent forms, especially for larger system. The purpose of this mini-symposium is to provide a platform for exchanging the recent developments on the numerical methods and theories for eigenvalue problems or equivalent forms arising in electronic structure calculations, and exploring the topic of further research and collaborations.

**Organizer(s) :** Huajie Chen (Beijing Normal University), Xiaoying Dai (Academy of Mathematics and Systems Science, CAS), Xin Liu (Academy of Mathematics and Systems Science, CAS), Yuzhi Zhou ( Institute of Applied Physics and Computational Mathematics)

**Classification :** 35Q55, 65N25, 81Q05,

**Minisymposium Program :**


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00969 (1/3) : 4C @G709 [Chair: Xiaoying Dai]

## [04472] Recent Advances in Self-Consistent-Field Iterations for Solving Eigenvector-Dependent Nonlinear Eigenvalue Problems

**Format :** Talk at Waseda University

**Author(s) :** Zhaojun Bai (University of California, Davis)

**Abstract :** Much like the power method for solving linear eigenvalue problems, self-Consistent-Field (SCF) iteration is a gateway algorithm to solve eigenvector-dependent nonlinear eigenvalue problems such as ones arising from electronic structure calculations. The SCF was introduced in computational physics back in the 1950s. In this talk, from numerical linear algebra perspective, we present recent advances in the SCF, such as sharp estimation of convergence rate and geometry interpretation of the SCF for a class of NEPs.

## [04337] Kohn-Sham GGA Models and Their Approximations

**Format :** Talk at Waseda University

**Author(s) :** Aihui Zhou (Academy of Mathematics and Systems Science, Chinese Academy of Sciences)

**Abstract :** In this presentation, I will talk about the finite dimensional approximations of Kohn-Sham GGA models, which are often used in electronic structure calculations. I will show the convergence of the finite dimensional approximations and present the a priori error estimates for ground state energy and solution approximations.

## [04173] Model and data driven electromagnetic inverse problems with optimal transport

**Format :** Online Talk on Zoom

**Author(s) :** Yanfei Wang (Institute of Geology and Geophysics, Chinese Academy of Sciences)

**Abstract :** Electromagnetic inverse problems have important applications in non-destructive testing and evaluation of materials. By using electromagnetic measurements to probe the properties of materials like metals and composites, researchers can gain insight into the structural integrity, conductivity, and other important

properties of these materials. In this study, we consider application of electromagnetic inverse problems in geophysics, i.e., using electromagnetic measurements to study the composition and structure of the Earth's subsurface. We propose a new attempt to use the probability metric (Wasserstein metric) for electromagnetic inversion. This lays the foundation for the future application of probability metric type of methods to large-scale electromagnetic inversion. In addition, data driven electromagnetic inverse problems will be also addressed.

## [05566] Porting Quantum ESPRESSO Eigensolvers on GPUS

**Format :** Talk at Waseda University

**Author(s) :** Stefano de Gironcoli (SISSA - Trieste)

**Abstract :** I will report on the effort by the Quantum ESPRESSO developing team regarding the porting of the main iterative eigensolvers employed in the solution the Kohn-Sham self-consistent equations in electronic structure applications to new hybrid hardware architectures including both CPUS and GPUS chips. Directions for future developments will be briefly outlined.

00969 (2/3) : 4D @G709 [Chair: Huajie Chen]

## [05006] An efficient LOBPCG solver for Kohn-Sham solution

**Format :** Talk at Waseda University

**Author(s) :** Guanghui Hu (University of Macau)

**Abstract :** In this talk, an efficient implementation of the LOBPCG solver in the self-consistent field iteration for the Kohn-Sham solution is introduced. It is found that in an  $h$ -adaptive finite element framework, the precondition in the LOBPCG method plays an important role to guarantee the fast convergence of the solver. Several choices are introduced, and the comparison of the performance among those choices will be demonstrated in detail.

## [03997] Sampling-based approaches for multimarginal optimal transport problems with Coulomb cost

**Format :** Talk at Waseda University

**Author(s) :** Yukuan Hu (Academy of Mathematics and Systems Science, Chinese Academy of Sciences)Mengyu Li (Renmin University of China)Xin Liu (Academy of Mathematics and Systems Science, Chinese Academy of Sciences)Cheng Meng (Renmin University of China)

**Abstract :** The multimarginal optimal transport problem with Coulomb cost find applications in understanding strongly correlated systems. We develop for its Monge-like reformulation novel methods that favor highly scalable subiteration schemes and avoid the full matrix multiplications in the existing ones. Convergence properties are built on the random matrix theory. For large-scale global resolution, we embed the proposed methods into a grid refinements-based framework. The numerical results corroborate the effectiveness and better scalability of our approach.

## [03145] A mixed precision LOBPCG algorithm

**Format :** Online Talk on Zoom

**Author(s) :** Daniel Kressner (EPF Lausanne)Yuxin Ma (Fudan University)Meiyue Shao (Fudan University)

**Abstract :** The LOBPCG algorithm is a popular approach for computing a few smallest eigenvalues of a large Hermitian positive definite matrix. We propose a mixed precision variant of LOBPCG that uses a (sparse) Cholesky factorization computed in lower precision as the preconditioner. We carry out a rounding error and convergence analysis of PINVIT, a simplified variant of LOBPCG. Our theoretical results predict and our numerical experiments confirm that the impact on convergence remains marginal.

## [04317] An extended plane wave framework for the electronic structure calculations of twisted bilayer material systems

**Format :** Online Talk on Zoom

**Author(s) :** Yuzhi Zhou Xiaoying Dai (Academy of Mathematics and Systems Science, Chinese Academy of Sciences)Aihui Zhou (Academy of Mathematics and Systems Science, Chinese Academy of Sciences)

**Abstract :** In this talk, we introduce extensions of our PW framework for the practical electronic calculations of twisted bilayer material systems in the following aspects: (1) a tensor-produced basis set with PWs in the incommensurate dimensions and localized functions in z direction, (2) the practical application of our newly developed cutoff techniques, and (3) a quasi-band structure picture under the small twisted angles and weak interlayer coupling limits. With (1) and (2), we have remarkably reduced the dimensions of hamiltonian matrix,

which makes the electronic structure calculations of twisted bilayer 2D material systems affordable to most modern computers. And (3) helps us better organize the calculations as well as understand results. We further use the linear TGB system with magic twisted angles as numerical examples. We have reproduced the famous flat bands with key features in good quantitative with other theoretical and experimental results. In terms of efficiency, our framework has much less computational cost compared to the commensurate cell approximations. While it is also more extendable compared to the traditional model hamiltonians and tight binding calculations. Lastly, nonlinear terms like Hartree energy and exchange-correlation energy can be readily included in the framework thus more effective and accurate DFT calculations of incommensurate 2D material systems can be expected in the near future.

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00969 (3/3) : 4E @G709 [Chair: Yuzhi Zhou]

## [04226] Grassmann Extrapolation of Density Matrices for Born–Oppenheimer Molecular Dynamics

**Format :** Online Talk on Zoom

**Author(s) :** Benjamin Stamm (University of Stuttgart)

**Abstract :** Born–Oppenheimer molecular dynamics (BOMD) is a powerful but expensive technique. We show how converged densities from previous DFT-calculations in the trajectory can be used to extrapolate a new guess for the SCF-iterations. We apply the method to real-life, multiscale, polarizable QM/MM BOMD simulations, showing that sizeable performance gains can be achieved. This is joint-work with É. Polack, G. Dusson and F. Lipparini.

## [04929] Applications of Atomic Cluster Expansion in Electronic Structure Calculations

**Format :** Online Talk on Zoom

**Author(s) :** Liwei Zhang (University of British Columbia)

**Abstract :** Nonlinear eigenvalue problems are quite typical in the field of electronic structure calculations. For decades, people tended to solve them by the so-called self-consistent field iterations method, which suffers from both convergence and numerical efficiency. In this talk, we will introduce a generalized Atomic Cluster Expansion (ACE) framework, which provides a complete and symmetry-preserving basis for approximating equivariant properties, to give rise to a way to skip the self-consistent procedure. We will also cover some potential applications of ACE in the context of post-DFT electronic structure calculation models.

## [04280] Numerical Analysis of the Operator Modification Approach for the Calculation of Band Diagrams of Crystalline Materials

**Format :** Online Talk on Zoom

**Author(s) :** Eric Cancès (CERMICS, École des Ponts and Inria Paris) Muhammad Hassan (Laboratoire Jacques-Louis Lions, Sorbonne Université) Laurent Vidal (CERMICS, École des Ponts and Inria Paris)

**Abstract :** In solid-state physics, electronic properties of crystalline materials are often described by the spectrum of periodic Schrödinger operators. Due to Bloch's theorem, the numerical computation of quantities of interest involves computing integrals over the Brillouin zone of energy bands, which are piecewise smooth, periodic functions obtained by solving a parametrized elliptic eigenvalue problem. Classic discretization strategies for resolving these eigenvalue problems produce approximate energy bands that are either non-periodic or discontinuous, both of which cause difficulties when employing numerical quadrature.

We present here an alternative discretization strategy based on an ad hoc operator modification approach. We derive a priori error estimates for the resulting energy bands and we show that these bands are periodic and can be made arbitrarily smooth (away from band crossings) by adjusting suitable parameters in the operator modification approach. We also present numerical experiments involving a toy model in 1D, graphene in 2D, and silicon in 3D to validate our theoretical results and showcase the efficiency of the operator modification approach.

# [00970] High Performance Linear Algebra Software toward Extreme Heterogeneity

## Session Time & Room :

00970 (1/2) : 4C (Aug.24, 13:20-15:00) @G305

00970 (2/2) : 4D (Aug.24, 15:30-17:10) @G305

## Type : Proposal of Minisymposium

**Abstract :** Today, the leadership High Performance Computing (HPC) systems accommodates exa-flops capability through massive parallelism from thousands of heterogeneous compute nodes. This poses a huge challenge for math library developers to derive scalable performance. This heterogeneity trend is likely to continue and it is anticipated that future computing systems could have multiple of accelerators or special processing options to accommodate a variety of application needs. This poses a new challenge for handling multiple types of computing node architectures. In this session, we will discuss the latest research on implementing linear algebra libraries for extreme scale heterogeneous computing systems.

**Organizer(s) :** Keita Teranishi and Pedro Valero Lara

**Classification :** 15-04, 68-04, 68VXX

## Minisymposium Program :

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00970 (1/2) : 4C @G305 [Chair: Keita Teranishi]

## [03921] Using the StarPU task-based runtime system for heterogeneous platforms as the core engine for a linear algebra software stack.

**Format :** Talk at Waseda University

**Author(s) :** Olivier Aumage (Inria)

**Abstract :** StarPU is a runtime system developed by Team STORM at Inria in Bordeaux, France, to support computing platforms based on heterogeneous architectures composed of combination of CPUs, GPUs and FPGAs. This talk will present how the Sequential Task Flow programming model offered by StarPU is being used to build a scalable, comprehensive linear algebra software stack for heterogeneous supercomputers.

## [04285] A Look at the Future of High-Performance Linear Algebra with DPLASMA and PaRSEC

**Format :** Online Talk on Zoom

**Author(s) :** george bositca (The University of Tennessee)

**Abstract :** This talk will focus on the dataflow programming to address some of the linear algebra challenges. I will focus in particular on two open-source projects, the PaRSEC runtime and the DPLASMA dense linear algebra library, and discuss the programming approach, the handling of heterogeneity and the opportunities to cover a large spectrum of linear algebra needs.

## [04413] Multiple- and Mixed-Precision BLAS with C++ Template

**Format :** Talk at Waseda University

**Author(s) :** Toshiyuki Imamura (RIKEN Center for Computational Science) Daichi Mukunoki (RIKEN Center for Computational Science) Atsushi Suzuki (RIKEN Center for Computational Science)

**Abstract :** We propose a new design for BLAS that can handle multiple- and mixed-precision computations. Our templated mixed-precision BLAS (tmBLAS) addresses weaknesses in existing BLAS by decoupling the data types of each operand and operator using C++ generic programming, with explicit descriptions of operators and type-castings. We demonstrate a prototype implementation that instantiates routines with FP{16, 32, 64, 128}, and DD data types with those operations in one level with higher precision than the data precision.

## [05194] MatRIS: A Scalable and Performance Portable Math Library for Heterogeneous and Multi-Device Systems based on the IRIS Runtime

**Format :** Talk at Waseda University

**Author(s) :** Keita Teranishi (Oak Ridge National Laboratory) Pedro Valero-Lara (Oak Ridge National Laboratory)

**Abstract :** Vendor libraries are tuned for one architecture and are not portable to others. Moreover, these lack support for heterogeneity and multi-device computation orchestration. We introduce MatRIS, a scalable and performance portable library for sparse/dense BLAS/LaPACK operations to address these challenges. MatRIS separates linear algebra algorithms and vendor libraries by using IRIS runtime. Such abstraction makes the implementation completely agnostic to the vendor libraries/architectures, providing high programming productivity. We demonstrate that MatRIS can fully utilize different multi-device heterogeneous systems, achieving high performance and scalability on three heterogeneous systems, Summit (#5 TOP500), Frontier (#1 TOP500), and CADES with four NVIDIA A100 GPUs and four AMD MI100 GPUs. A detailed performance study is presented for sparse and dense LU factorization where MatRIS provides a speedup of up to 8 $\times$  from the previous version of the library (LaRIS). Along with better scalability, MatRIS provides competitive and even better performance than vendor libraries.

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00970 (2/2) : 4D @G305 [Chair: Keita Teranishi]

## [05190] Responsibly Reckless Matrix Algorithms for HPC Scientific Applications

**Format :** Talk at Waseda University

**Author(s) :** Hatem Ltaief (KAUST)

**Abstract :** Referred to by Jack Dongarra, the 2021 ACM Turing Award Laureate, as “responsibly reckless” matrix algorithms, we highlight the implications of mixed-precision (MP) computations for HPC applications. Reducing precision comes at the price of trading away some accuracy for performance (reckless) but in noncritical segments of the workflow (responsible) so that the accuracy requirements of the application can still be satisfied. We illustrate the MP impact on seismic imaging, climate/environment geospatial predictions, and computational astronomy.

## [04598] A scalable multi-GPU approach for solving H2-approximated dense linear systems

**Format :** Talk at Waseda University

**Author(s) :** Qianxiang Ma (Tokyo Institute of Technolgy) Rio Yokota (Global Scientific Information and Computing Center, Tokyo Institute of Technology)

**Abstract :** In this talk, we present a novel approach for directly solving a dense linear system emerged from 3-D geometry approximated using  $\mathcal{H}^2$ -matrices. From the pre-compressing the fill-ins, we are able to ULV-factorize and apply forward and backward substitution in an entirely parallel manner by batched BLAS/LAPACK operations on GPUs. Using 512 NVIDIA V100 GPUs, we are able to factorize a matrix of N=29,242,368 under 1 second, utilizing 0.808 PFLOPS/s of performance.

## [05233] Towards a Unified Micro-kernel Abstraction for GPU Linear Algebra

**Format :** Talk at Waseda University

**Author(s) :** Vijay Thakkar (NVIDIA | Georgia Tech) Richard Vuduc (Georgia Tech)

**Abstract :** We have created a micro-kernel abstraction for GPUs robust enough to represent the tensor core and data movement operations from NVIDIA GPU architectures spanning Maxwell all the way to Hopper. In this talk, we discuss how CuTe layouts and layout algebra allow us to uniformly represent GPU architecture specific operations in a consistent programming model regardless of the threads and data they operate upon to build CUTLASS 3.x's core abstractions.

# [00974] Finite element complexes and multivariate splines

**Session Time & Room :**

00974 (1/3) : 3D (Aug.23, 15:30-17:10) @E703

00974 (2/3) : 3E (Aug.23, 17:40-19:20) @E703

00974 (3/3) : 4C (Aug.24, 13:20-15:00) @E703

**Type :** Proposal of Minisymposium

**Abstract :** Differential complexes encode important structures in a wide range of problems, and there has been a surge of interest in discretizing these complexes. Examples include the de-Rham complex, the elasticity complex, and, more recently, other BGG complexes. Algebraic and differential geometric structures play an important role in the construction of finite elements and multivariate splines. This mini-symposium aims to bring together researchers to discuss recent progress in the construction of discrete complexes and the emerging connections between algebra, geometry and discretization.

**Organizer(s) :** Kaibo Hu, Nelly Villamizar

**Classification :** 65M60, 65D07, 65M70, 14Q99, 14F40, finite elements, splines, exterior calculus, applied algebraic geometry

**Minisymposium Program :**

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00974 (1/3) : 3D @E703 [Chair: Kaibo Hu]

## [02331] A polytopal exterior calculus framework

**Format :** Online Talk on Zoom

**Author(s) :** Francesco Bonaldi (University of Perpignan) Daniele Antonio Di Pietro (University of Montpellier) Jerome Droniou (Monash University) Kaibo Hu (University of Oxford)

**Abstract :** For  $\Omega \subset \mathbf{R}^n$ , the de Rham complex of differential forms

$$0 \rightarrow H\Lambda^0(\Omega) \xrightarrow{d} H\Lambda^1(\Omega) \xrightarrow{d} \cdots \xrightarrow{d} H\Lambda^n(\Omega) \xrightarrow{d} 0 \quad (1)$$

is essential to establish the well-posedness of certain PDE models; developing discrete versions of this complex is a key for designing robust schemes for these models. We will present two such discrete complexes, inspired by the DDR and VEM approaches, of arbitrary order, and applicable on generic meshes. Compared to FEEC, these complexes benefit from the flexibility and high-level construction of polytopal methods.

## [05349] Finite Element Complex

**Format :** Talk at Waseda University

**Author(s) :** Long Chen (University of California at Irvine) Xuehai Huang (Shanghai University of Finance and Economics)

**Abstract :** This presentation provides an overview of finite element complex construction, showcasing the finite element de Rham complex through a geometric decomposition method. The construction is extended to additional finite element complexes, such as the Hessian complex, elasticity complex, and divdiv complex, using the Bernstein-Gelfand-Gelfand (BGG) framework.

The resulting finite element complexes hold potential applications in numerical simulations for the biharmonic equation, linear elasticity, general relativity, and other geometry-related PDEs.

## [05423] Diagram chases yielding discrete elasticity complexes

**Format :** Talk at Waseda University

**Author(s) :** Jay Gopalakrishnan (Portland State University)

**Abstract :** Differential complexes have shed new insight into the finite elements in recent years. This talk is devoted to the elasticity complex, which provides an example of how complicated exact sequences of spaces can be built from simple ones. Lining up two simpler complexes, we start by performing a "diagram chase", which often goes

by the name of Bernstein-Gelfand-Gelfand resolution. The purpose of this talk is to outline a few cases where this process can be perfectly mimicked at the discrete level. The earliest example in three-dimensions is on mesh of macroelements of Alfeld splits, facilitated by the understanding of supersmoothness from research into splines. Other emerging constructions will also be touched upon. (Parts of the talk contain results obtained jointly with S. Christiansen, S. Gong, J. Guzman, K. Hu, and M. Nielan.)

## [03116] Nonconforming finite element exterior calculus

**Format :** Talk at Waseda University

**Author(s) :** Shuo Zhang (Academy of Mathematics and Systems Science, Chinese Academy of Sciences)

**Abstract :** A family of nonconforming finite element complexes are presented for n-dimensional de Rham complexes,  $n \geq 2$ . Particularly, the n-dimensional Crouzeix-Raviart elements are used to discretize the space of 0 forms. These finite element spaces are generally not constructed by Ciarlet's triples, and can be viewed as nonconforming splines. New theories are presented so that many basic properties of the finite element spaces and complexes can be established.

00974 (2/3) : 3E @E703 [Chair: Nelly Villamizar]

## [05444] Bounds on smooth spline spaces

**Format :** Online Talk on Zoom

**Author(s) :** Henry Schenck (Auburn University)Michael Stillman (Cornell University)Beihui Yuan (Swansea University)

**Abstract :** For a planar simplicial complex  $\Delta$  contained in  $R^2$ , Schumaker proved that a lower bound on the dimension of the space  $C^r_k(\Delta)$  of planar splines of smoothness  $r$  and polynomial degree at most  $k$  on  $\Delta$  is given by a polynomial  $P_{\Delta}(r,k)$ , and Alfeld-Schumaker showed this polynomial gives the correct dimension when  $k \geq 4r+1$ . We prove that the equality  $\dim C^r_k(\Delta) = P_{\Delta}(r,k)$  cannot hold in general for  $k \leq (22r+7)/10$ .

## [04982] Conforming Finite Element Methods with Arbitrary Smoothness in Any Dimension

**Format :** Talk at Waseda University

**Author(s) :** Jun Hu (Peking University)Ting Lin (Peking University)Qingyu Wu (Peking University)

**Abstract :** This talk proposes a construction of  $C^r$  conforming finite element spaces with arbitrary  $r$  in any dimension. It is shown that if  $k \geq 2^d r + 1$  the space  $P_k$  of polynomials of degree  $\leq k$  can be taken as the shape function space of  $C^r$  finite element spaces in  $d$  dimensions. This is the first work on constructing such  $C^r$  conforming finite elements in any dimension in a unified way.

## [03133] An algebraic framework for geometrically continuous splines

**Format :** Talk at Waseda University

**Author(s) :** Angelos Mantzaflaris (Inria at Universite Cote d'Azur, Sophia Antipolis, France)Bernard Mourrain (Inria at Universite Cote d'Azur, Sophia Antipolis, France)Nelly Villamizar (Swansea University)Beihui Yuan (Swansea University)

**Abstract :** Geometrically continuous splines are piecewise polynomials defined on a collection of patches stitched together through transition maps. In this talk, we introduce an algebraic framework to study geometrically continuous splines. This framework enables us to use algebraic tools to analyze the dimension of spline spaces, and to present a new algorithm to construct bases using algebraic methods. This talk is based on a joint work with Angelos Mantzaflaris, Bernard Mourrain and Nelly Villamizar.

## [05200] Multivariate spline functions on "oranges"

**Format :** Talk at Waseda University

**Author(s) :** Nelly Villamizar (Swansea University)Maritza Sirvent (The Ohio State University)Tatyana Sorokina (Towson University)Beihui Yuan (Swansea University)Michael DiPasquale (University of South Alabama)

**Abstract :** A spline is a piecewise polynomial function defined on a partition of a real domain. Splines play an important role in many areas such as finite elements, computer-aided design, and data fitting.

In the talk, we will focus on splines defined on "oranges" which are partitions composed of a finite number of simplices of the same dimension that share one common lower dimensional face. For any fixed maximal polynomial degree and minimum order of global smoothness, we prove that the dimension of the spline space on an orange can be computed as a sum of the dimension of spline spaces on simpler lower-dimensional partitions. The examples and results in the talk combine both Bernstein-Bézier methods for splines and algebraic tools.

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00974 (3/3) : 4C @E703 [Chair: Kaibo Hu]

## [05202] The strain Hodge Laplacian and discretisation of the incompatibility operator

**Format :** Talk at Waseda University

**Author(s) :** Francis Raul Anthony Aznaran (University of Oxford)Kaibo Hu (University of Oxford)

**Abstract :** Motivated by the physical relevance of many Hodge Laplace PDEs from the FEEC, we analyse the Hodge Laplacian arising from the strain space  $H(\text{inc}; \mathbb{R}_{\text{sym}}^{d \times d})$ ,  $\text{inc} := \text{rot} \circ \text{rot}$ , in the elasticity complex. We propose an adaptation of  $C^0$ -interior penalisation for the incompatibility, using the Regge element to discretise the strain. Building on pioneering work by van Goethem, we discuss promising connections between functional analysis of the inc operator and Kröner's intrinsic theory of defect elasticity.

## [02874] Nonconforming finite elements for the Brinkman Problems and Quad-curl Problems on Cubical Meshes

**Format :** Talk at Waseda University

**Author(s) :** Qian Zhang (Michigan Technological University)

**Abstract :** In this talk, I will present two families of nonconforming elements on cubical meshes: one for the quad-curl problem and the other for the Brinkman problem. The element for the quad-curl problem is the first nonconforming element on cubical meshes. The element for the Brinkman problem can yield a uniformly stable finite element method with respect to the parameter  $\nu$ . The lowest-order elements for the quad-curl and the Brinkman problems have 48 and 30 degrees of freedom, respectively. The two families of elements, as a nonconforming approximation to  $H((\text{gradcurl}))$  and  $H^1$ , can form a discrete Stokes complex together with the Lagrange element and the DG element.

## [05642] Distributional finite element BGG complexes

**Format :** Talk at Waseda University

**Author(s) :** Jay Gopalakrishnan (Portland State University)Kaibo Hu (University of Oxford)Ting Lin (Peking University)Joachim Schöberl (TU Wien)Qian Zhang (Michigan Technological University)

**Abstract :** Distributional finite elements generalize classical concepts by allowing measures (Dirac deltas) as shape functions. Distributional elements were used to derive equilibrated residual error estimators (Braess, Schöberl 2008) and discretization of the stress-displacement formulation of linear elasticity (Pechstein, Schöberl 2011, TDNNS). Regge calculus from discrete relativity can be interpreted as a finite element version of metric with distributional curvature (Christiansen 2008). In this talk, we review the concept of distributional elements and discuss progress in discretizing Bernstein-Gelfand-Gelfand (BGG) diagrams and sequences.

## [00975] Data-driven methods for learning mathematical models

**Session Time & Room :** 5D (Aug.25, 15:30-17:10) @G703

**Type :** Proposal of Minisymposium

**Abstract :** Mathematical models are important tools helping people understand scientific phenomena in many disciplines. Recent advances in technologies make it easier to collect huge amounts of data, which offers new opportunities on data-driven methods for the identification of mathematical models behind a phenomenon. This minisymposium focuses on learning mathematical models from an observed data set. Topics in this field include identification of governing equations, reconstruction of certain functions in an equation, and learning operators between input and output spaces. Recently, there have been interesting developments in this field, varying from problem formulations, efficient solvers, techniques on improving robustness to theoretical analysis. This minisymposium brings together researchers to discuss recent advances, challenges and applications in this field.

part\_2

**Organizer(s)** : Yuchen He, Hao Liu

**Classification** : 35RXX, 65ZXX, 37MXX, 65MXX, differential equation and operator learning

**Minisymposium Program :**

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00975 (1/1) : 5D @G703 [Chair: Hao Liu]

## [05503] Recent Advances in Weak Form-Based System Identification

**Format** : Online Talk on Zoom

**Author(s)** : David Bortz (University of Colorado - Boulder) Daniel Messenger (University of Colorado - Boulder)

**Abstract** : Recent advances in data-driven modeling approaches have proven highly successful in a wide range of fields in science and engineering. In this talk, I will present our weak form methodology which has proven to have surprising performance properties. After describing our equation learning (WSINDy) and parameter estimation (WENDy) algorithms, I will discuss applications to several benchmark problems to illustrate the computational efficiency, noise robustness, and modest data needs.

## [05502] Identification of variable coefficient PDEs using group projected subspace pursuit

**Format** : Online Talk on Zoom

**Author(s)** : Yuchen He (Shanghai Jiao Tong University) Sung Ha Kang (Georgia Institute of Technology) Wenjing Liao (Georgia Institute of Technology) Hao Liu (Hong Kong Baptist University) Yingjie Liu (Georgia Institute of Technology)

**Abstract** : We propose a novel scheme, GP-IDENT, for identifying variable coefficient PDEs from noisy observations of single solution trajectories. To effectively solve the associated feature selection problems, we designed a group projected subspace pursuit (GPSP) algorithm, which is also suitable for general feature selection problems with group structure. We will provide examples to show that GP-IDENT can successively identify many non-linear high-order PDEs, and its effectiveness is also justified via comparisons with state-of-the-art methods.

## [05509] How much can one learn a PDE from its solution?

**Format** : Talk at Waseda University

**Author(s)** : Yimin Zhong (Auburn University) Hongkai Zhao (Duke University) Yuchen He (Shanghai Jiao Tong University)

**Abstract** : In this work we study a few basic questions for PDE learning from observed solution data. Using various types of PDEs, we show 1) how the approximate dimension (richness) of the data space spanned by all snapshots along a solution trajectory depends on the differential operator and initial data, and 2) identifiability of a differential operator from solution data on local patches. Then we propose a consistent and sparse local regression method (CaSLR) for general PDE identification. Our method is data driven and requires minimal amount of local measurements in space and time from a single solution trajectory by enforcing global consistency and sparsity.

## [05246] Learning Koopman Operators that Generalize Well

**Format** : Online Talk on Zoom

**Author(s)** : Bethany Lusch (Argonne National Laboratory)

**Abstract** : The Koopman operator is a way to represent a nonlinear dynamical system as a globally linear system. However, the linear system is infinite-dimensional, and the representation is difficult to find. Much recent research is on data-driven methods to approximate the Koopman operator. However, finding an approximation that generalizes well for a large region without finely sampling the space can be challenging. We explore learning a Koopman operator that can generalize well given limited data.

# [00977] Recent advances on sparse optimization: algorithms and applications

**Session Time & Room** : 5C (Aug.25, 13:20-15:00) @A206

**Type :** Proposal of Minisymposium

**Abstract :** Sparse optimization arises from various application problems in statistics and machine learning. In the past decades, the well-known Lasso model and its variants have been extensively studied, and many efficient methods have been well explored correspondingly. Nevertheless, efficient methods for solving more and more difficult models involving sparse structures are still under explored. Considering the high dimension of the application problems, it is important to highly utilize their structures thus to obtain efficient algorithms. In this minisymposium, we focus on recent development of the algorithms and applications of the modern sparse optimization.

**Organizer(s) :** Lei Yang, Tianxiang Liu

**Classification :** 90C26, 90C30, 65K05

**Minisymposium Program :**

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00977 (1/1) : 5C @A206 [Chair: Tianxiang Liu]

## [02162] Asymptotically Consistent Linear Convergence Rate of the Randomized Sparse Kaczmarz Method

**Format :** Talk at Waseda University

**Author(s) :** Liang Chen (Hunan University)

**Abstract :** The sparse Kaczmarz method has drawn much attention from researchers in recent years. This is mainly due to its capability of producing sparse solutions to linear systems, which is a core problem of many applications in the big-data era, such as sparse signal recovery and image processing. This method was shown to be linearly convergent in 2019. However, the convergence rate is not consistent with the well-known convergence rate of the randomized Kaczmarz method. In this work, we try to fix this gap by proposing an asymptotically consistent linear convergence rate for the former.

## [02234] A difference-of-convex algorithm for sparse support vector machines in high dimensions

**Format :** Talk at Waseda University

**Author(s) :** Ning Zhang (Dongguan University of Technology)

**Abstract :** The support vector machine (SVM) is a popular and powerful technique for binary classification. We consider the penalized SVM with a class of difference-of-convex penalties. We show that the difference-of-convex algorithm is guaranteed to produce an oracle estimator in two iterations if the solution to L1-norm SVM is selected as the initial estimator. We further prove that the d.c. algorithm for SCAD/MCP penalized SVM converges to a d-stationary point with local linear convergence rate.

## [01567] Frank-Wolfe type methods for a class of nonconvex inequality-constrained problems

**Author(s) :** Liaoyuan Zeng (Zhejiang University of Technology) Yongle Zhang (Sichuan Normal University) Guoyin Li (University of New South Wales) Ting Kei Pong (The Hong Kong Polytechnic University)

**Abstract :** The Frank-Wolfe method and its variants, which implement efficient linear oracles for minimizing smooth functions over compact convex sets, form a prominent class of projection-free first-order methods. In this talk, we extend the Frank-Wolfe method and its away-step variant for minimizing a smooth function over a possibly nonconvex compact set, based on our new generalized linear oracles. We discuss convergence and present numerical performance of our nonconvex Frank-Wolfe type methods for solving matrix completion problems.

# [00980] Recent Advances in Applied Mathematics including adopting machine learning and deep learning

**Session Time & Room :** 1D (Aug.21, 15:30-17:10) @E504

**Type :** Proposal of Minisymposium

**Abstract :** Applied mathematics is the field of mathematical methods and statistical reasoning to solve practical problems of a scientific or decision-making nature in a variety of subjects, engineering, medicine, physical and biological sciences. In particular, Industrial mathematics is one of the fastest-growing branches in applied mathematics and plays a growing role in developing robotics and automation systems, mechanical engineering, medicine, and others. It is concerned with developing and finding the most efficient mathematical methods to solve problems arising in recent.

This session consists of recent research trends on applied mathematics, numerical analysis to find optimal solutions, and statistical methodology for uncertainty inference including machine learning (deep learning) applications.

**Organizer(s) :** Taeyoung Ha, Soon-Sun Kwon

**Classification :** 62P10, 65K10, Deep learning

**Minisymposium Program :**

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00980 (1/1) : 1D @E504 [Chair: Soon-Sun Kwon]

## [01658] A hybrid difference method and its postprocessings for second order elliptic problems

**Format :** Talk at Waseda University

**Author(s) :** Dongwook Shin (Ajou University)Youngmok Jeon (Ajou University)Eun-Jae Park (Yonsei University)

**Abstract :** In this talk, we investigate a new method, the hybrid difference method, proposed by S., Jeon, and Park (Appl. Math. Comput., 2022), for second order elliptic problems. The hybrid difference method is a finite difference method that is based on the hybrid discontinuous Galerkin method introduced by Jeon and Park (SINUM, 2010). The HD method allows arbitrarily high-order approximations, and the local conservation property holds. The HD method allows arbitrarily high-order approximations, and satisfies the local conservation property. Additionally, it can significantly reduce the global degrees of freedom by the static condensation via Schur complement similar to the HDG method. In the recent work, we have extended and improved the HD method by introducing additional conditions. This new generalized method can be seen as the method introduced by Jeon, Park, and S. (Comput. Methods Appl. Math., 2017) with the addition of a simple postprocessing. To increase computational efficiency, we also introduce a residual type error estimator that allows for the use of adaptive algorithms. The proposed method can be extended to more complex domain geometries through simple modifications, although the local conservation property may not hold in these cases and thus requires further postprocessing. Several numerical experiments are presented to show the performance of the proposed method, which support our theoretical findings.

## [05287] Predicting Thermoelectric Material Properties using Machine Learning

**Format :** Talk at Waseda University

**Author(s) :** YunKyong Hyon (National Institute for Mathematical Sciences)

**Abstract :** According to the development of machine learning technologies, the application of machine learning is already very active in all research areas. Material design requires a lot of calculation and computer resources in its classical process, but the process and period of material development can be shortened by using machine learning methodologies. We present a machine learning model that predicts the properties of materials required for the development of thermoelectric materials and its performance.

## [05338] Classification of respiratory sounds using deep learning methods

**Format :** Talk at Waseda University

**Author(s) :** Sunju Lee (National Institute for Mathematical Sciences (NIMS))

**Abstract :** Auscultation with a stethoscope has been an essential part of diagnosing patients with respiratory diseases and providing first aid. However, accurate interpretation and diagnosis of auscultation sounds relies on the expertise of clinicians, so it is important to develop an artificial intelligence-based diagnosis support system using respiratory sounds. In this talk, we propose a deep-learning based classification model for respiratory sounds recorded in the clinical setting.

## [05339] Interpretable Classification for Multivariate Gait Analysis

**Format :** Talk at Waseda University

**Author(s) :** Soon-Sun Kwon (Department of Mathematics/Artificial Intelligence, Ajou University, South Korea)

**Abstract :** Motivated by gait data from both the normal and the cerebral palsy (CP) patients group with various gross motor function classification system (GMFCS) levels, we propose a multivariate functional classification method to investigate the relationship between kinematic gait measures and GMFCS levels. A sparse linear functional discrimination framework is utilized to achieve an interpretable prediction model. The method is generalized to handle multivariate functional data and multi-class classification. The method yields superior prediction accuracy and provides easily interpretable discriminant functions. And it will help clinicians to diagnose CP and assign an appropriate GMFCS level in a more consistent and mathematical evidence.

## [00981] Various Methods for the Analysis of PDEs

**Session Time & Room :** 5B (Aug.25, 10:40-12:20) @G709

**Type :** Proposal of Minisymposium

**Abstract :** There has been a strong interaction between classical analysis (theory of function spaces, harmonic analysis, geometric analysis, asymptotic analysis, real analysis, functional analysis, etc ) and nonlinear partial differential equations.

This minisymposium provides a forum to discuss the latest methods for the analysis of nonlinear partial differential equations arising in Mathematical Physics and to exchange ideas for further developments.

**Organizer(s) :** Vladimir Georgiev (University of Pisa, Waseda University), Tohru Ozawa (Waseda University)

**Classification :** 35Q55, 35L10, 46E35, 26D10, 42B37

**Minisymposium Program :**

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00981 (1/1) : 5B @G709 [Chair: Vladimir Georgiev]

## [03982] Carleson's problem for infinitely many fermions

**Format :** Talk at Waseda University

**Author(s) :** Neal Bez (Saitama University)

**Abstract :** Carleson's problem for the free Schrodinger equation is concerned with the minimal level of regularity that guarantees the solution converges to the initial data in an almost everywhere sense as time goes to zero. Here we consider a version of this problem for infinitely many particles.

## [05489] Stabilité results for the Sobolev inequality with computable constants and optimal behaviour

**Format :** Talk at Waseda University

**Author(s) :** Maria J. Esteban (CNRS and University Paris-Dauphine)

**Abstract :** In this talk I will present recent results concerning optimal quantitative stability properties for the Sobolev and logarithmic-Sobolev inequalities with computable constants. The result for the Gaussian version of the logarithmic Sobolev inequality is actually a corollary of the one for Sobolev. This is done, in an optimal manner, by a limiting argument in high dimensions.

This work is the result of a collaboration with J. Dolbeault, A. Figalli, R. Frank and M. Loss.

## [05451] Lifespan estimate for classical damped wave equations with some initial data

**Format :** Talk at Waseda University

**Author(s) :** Kazumasa FUJIWARA (Ryukoku university )Vladimir Georgiev (Pisa University)

**Abstract :** The lifespan estimate for the Cauchy problem of the semilinear classical damped wave equation is estimated when the Fourier 0th mode of the initial data is 0. In earlier works, the lifespan was estimated based on the magnitude of the Fourier 0th mode of the initial data. We will explore the lifespan estimate by considering the magnitude of the Fourier 1st and 2nd modes of the initial data instead of the 0th mode.

part\_2

## [05511] Blow-up for the 1d cubic NLS

**Format :** Talk at Waseda University

**Author(s) :** Luis Vega (BCAM-UPV/EHU)

**Abstract :** We consider the 1D cubic NLS on  $\mathbb{R}$  and prove a blow-up result for functions that are of borderline regularity, i.e.  $H^s$  for any  $s < -1/2$  for the Sobolev scale and  $L^\infty$  for the Fourier-Lebesgue scale. This is done by identifying at this regularity a certain functional framework from which solutions exit in finite time. This functional framework allows, after using a pseudo-conformal transformation, to reduce the problem to a large-time study of a periodic Schrödinger equation with non-autonomous cubic nonlinearity. The blow-up result corresponds to an asymptotic completeness result for the new equation. We prove it using Bourgain's method and exploiting the oscillatory nature of the coefficients involved in the time-evolution of the Fourier modes. Finally, as an application we exhibit singular solutions of the binormal flow. More precisely, we give conditions on the curvature and the torsion of an initial smooth curve such that the constructed solutions generate several singularities in finite time. This is a joint work with V. Banica, R. Luca, and N. Tzvetkov

## [00982] Partial Differential Equations in Fluid Dynamics

**Session Time & Room :**

00982 (1/3) : 1C (Aug.21, 13:20-15:00) @G405

00982 (2/3) : 1D (Aug.21, 15:30-17:10) @G405

00982 (3/3) : 1E (Aug.21, 17:40-19:20) @G405

**Type :** Proposal of Minisymposium

**Abstract :** This mini-symposium is aimed to bring together the leading experts as well as promising young researchers to present their recent results in partial differential equations with applications in fluid dynamics. Key topics focus on the most challenging open problems in the area such as global regularity, uniqueness of solutions, singular limits, boundary layers behavior, and free boundary problems, etc. It also provides a premier interdisciplinary forum for senior and junior researchers to exchange their experiences in the study of partial differential equations. The talks will span from analysis through modeling and computation to applications of partial differential equations.

**Organizer(s) :** Yachun Li, Ming Mei, Shinya Nishibata, Ronghua Pan

**Classification :** 35-xx, 76-xx, partial differential equations, fluid mechanics

**Minisymposium Program :**

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00982 (1/3) : 1C @G405 [Chair: Shinya Nishibata]

## [04512] Two-Dimensional Riemann Problems: Transonic Shocks and Free Boundary Problems

**Format :** Online Talk on Zoom

**Author(s) :** Gui-Qiang George Chen (University of Oxford)

**Abstract :** We are concerned with global solutions of multidimensional Riemann problems for nonlinear hyperbolic systems of conservation laws, focusing on their global configurations and structures. We present some recent developments in the rigorous analysis of two-dimensional Riemann problems involving transonic shock waves and free boundary problems through several prototypes of hyperbolic systems of conservation laws and discuss some further M-D Riemann problems and related problems for nonlinear partial differential equations.

## [05347] Global stability of steady supersonic flow for 1D Compressible Euler system

**Format :** Talk at Waseda University

**Author(s) :** Jianli Liu (Shanghai University)

**Abstract :** It is more important to consider the stability of compressible flow with some physical effects. In this talk, we will give the global nonlinear stability of steady supersonic flows for one dimensional unsteady compressible

Euler systems with physical effect, such as a nonlinear damping representing frictions, heat transfer term or mass addition.

## [04192] Scaling limit of vortex dynamics on the filtered-Euler flow

**Format :** Talk at Waseda University

**Author(s) :** Takeshi Gotoda (Tokyo Institute of Technology)

**Abstract :** We consider weak solutions of the 2D filtered-Euler equations, which describe a regularized Euler flow. We show that, in the limit of the filtering scale, filtered weak solutions converge to weak solutions of the 2D Euler equations and an energy dissipation rate for the filtered weak solution converges to zero for initial vorticity in a certain class.

## [05331] Characteristic Decomposition for Hyperbolic System

**Format :** Talk at Waseda University

**Author(s) :** Wancheng Sheng (Shanghai University)

**Abstract :** In this talk, we show the method of characteristic decompositions for hyperbolic conservation laws. By this methods, we give some results on the multidimensional Riemann problems of compressible Euler equations.

00982 (2/3) : 1D @G405 [Chair: Ronghua Pan]

## [04072] Global Finite-Energy Solutions of the Compressible Euler-Poisson Equations for General Pressure Laws with Spherical Symmetry

**Format :** Talk at Waseda University

**Author(s) :** Feimin Huang (Academy of Mathematics and Systems Science, Chinese Academy of Science)

**Abstract :** We are concerned with global finite-energy solutions of the three-dimensional compressible Euler-Poisson equations with gravitational potential and general pressure law, especially including the constitutive equation of white dwarf stars. In this paper, we construct a global finite-energy solution with spherical symmetry of the Cauchy problem for the Euler-Poisson equations as the vanishing viscosity limit of the corresponding compressible Navier-Stokes-Poisson equations. The strong convergence of the vanishing viscosity solutions is achieved through the compensated compactness analysis and uniform estimates in  $L^p$  via several new main ingredients. A new key estimate is first established for the integrability of the density over unbounded domains independent of the vanishing viscosity coefficient. Then a special entropy pair is carefully designed via solving a Goursat problem for the entropy equation such that a higher integrability of the velocity is established, which is a crucial step. Moreover, the weak entropy kernel for the general pressure law and its fractional derivatives of the required order near vacuum ( $\rho = 0$ ) and far-field ( $\rho = \infty$ ) are carefully analyzed. Owing to the generality of the pressure law, only the  $W_{\text{loc}}^{-1,p}$ -compactness of weak entropy dissipation measures with  $p \in [1, 2]$  can be obtained; this is rescued by the equi-integrability of weak entropy pairs which can be established by the estimates obtained above, so that the div-curl lemma still applies. Finally, based on the above analysis of weak entropy pairs, the  $L^p$  compensated compactness framework for the compressible Euler equations with general pressure law is established. This new compensated compactness framework and the techniques developed in this paper should be useful for solving further nonlinear problems with similar features.

## [04789] Global-in-time quasi-neutral limit for a two-fluid Euler-Poisson system

**Format :** Talk at Waseda University

**Author(s) :** Yue-Jun Peng (Université Clermont Auvergne)

**Abstract :** We consider Cauchy problem for a two-fluid Euler-Poisson system where the single parameter is the Debye length. When the initial data are sufficiently close to constant equilibrium states, we show the uniform global existence of smooth solutions and justify the convergence of the system to compressible Euler equations with damping as the Debye length tends to zero. We also establish global error estimates of the solutions. A key step of the proof is to control the quasi-neutrality of the velocities by using a projection operator.

## [03623] A compressible two-fluid model with unequal velocities: existence and uniqueness

**Format :** Talk at Waseda University

**Author(s) :** Huanyao Wen (South China University of Technology)

**Abstract :** In this talk, we will introduce our recent works on the existence and uniqueness theory of a compressible two-fluid model with unequal velocities. The viscosity coefficients depend on the density functions, which can be degenerate.

## [04539] On the Stability of Outflowing Compressible Viscous Gas

**Format :** Talk at Waseda University

**Author(s) :** Yucong Huang (University of Edinburgh)Shinya Nishibata (Tokyo Institute of Technology)

**Abstract :** I will discuss the long-time stability of a spherically symmetric motion of outflowing isentropic and compressible viscous gas. The fluid occupies unbounded exterior domain, and it is flowing out from an inner sphere centred at the origin. In this talk, I will show that, for a large initial data, the solution will converge to the stationary solution as time goes to infinity. This is a joint work with S. Nishibata.

00982 (3/3) : 1E @G405 [Chair: Ming Mei]

## [04434] Hyperbolic Cattaneo-Approximation of the compressible Navier-Stokes-Fourier system

**Format :** Talk at Waseda University

**Author(s) :** Jiang Xu (Nanjing University of Aeronautics and Astronautics)

**Abstract :** We will talk about the Cattaneo-Chistov approximation of the compressible non-isentropic Navier-Stokes system in whole space. First, we establish a global well-posedness of the Navier-Stokes-Cattaneo-Christov system uniformly with respect to the relaxation parameter. Then we justify the strong convergence of the solution toward that of the compressible Navier-Stokes system, and the explicit convergence rates are also exhibited.

## [04767] Local regularity conditions on initial data for local energy solutions of the incompressible Navier-Stokes equations

**Format :** Talk at Waseda University

**Author(s) :** Hideyuki Miura (Tokyo institute of technology)Kyungkeun Kang (Yonsei university)Tai-Peng Tsai (University of British Columbia)

**Abstract :** We study the regular sets of local energy solutions to the Navier-Stokes equations in terms of conditions on the initial data. It is shown that if a weighted L<sub>2</sub> norm of the initial data is finite, then all local energy solutions are regular in a region confined by space-time hypersurfaces determined by the weight. This result refines and generalizes Theorems C and D of Caffarelli, Kohn and Nirenberg (1982).

## [04554] Sharp non-uniqueness of weak solutions to viscous fluids

**Format :** Talk at Waseda University

**Author(s) :** Yachun Li (Shanghai Jiao Tong University) Zirong Zeng (Shanghai Jiao Tong University)Deng Zhang (Shanghai Jiao Tong University)Peng Qu (Fudan University)

**Abstract :** In this talk, I will present our recent results about non-uniqueness of weak solutions to some viscous fluid models. For incompressible Navier-Stokes equations , we proved the sharp non-uniqueness of weak solutions at two endpoints of the Ladyženskaya-Prodi-Serrin (LPS) criteria even in hyper-viscous regime. For MHD equations, we prove the sharp non-uniqueness near one endpoint of the LPS condition. Furthermore, the strong vanishing viscosity and resistivity result is obtained, it yields the failure of Taylor's conjecture along some sequence of weak solutions. For hypo-viscous compressible Navier-Stokes equations, we prove that there exist infinitely many different weak solutions with the same initial data. This provides the first non-uniqueness result of weak solutions to viscous compressible fluid. Our proof are based on the spatial-temporal intermittent convex integration scheme. These are joint works with Yachun Li, Peng Qu and Deng Zhang.

## [05340] On controllability of the incompressible MHD system

**Format :** Talk at Waseda University

**Author(s) :** Yaguang Wang (Shanghai Jiao Tong University)

**Abstract :** In this talk, we shall introduce our recent study on the controllability of the initial boundary value problem for the incompressible magnetohydrodynamic systems. For the two-dimensional ideal incompressible MHD system, we obtained the global exact controllability by using the return method, and for the two- and three-dimensional viscous MHD systems with coupled Navier slip boundary condition, we deduced the global approximate controllability. This is a joint work with Manuel Rissel.

## [00988] Treatment of infinity and finite-time singularities in differential equations

**Session Time & Room :**

00988 (1/2) : 1C (Aug.21, 13:20-15:00) @G402

00988 (2/2) : 1D (Aug.21, 15:30-17:10) @G402

**Type :** Proposal of Minisymposium

**Abstract :** Finite-time singularities arise in various problems in differential equations and have been ones of the most important issues towards the comprehensive understanding of the global nature of systems for decades.<sup>[1]</sup> In recent years, various universal machineries from geometry, dynamical systems and numerical analysis have been proposed and applied to unraveling wide variety of finite-time singularities, as well as appropriate treatments of infinity, and the common nature among them.

This symposium aims at sharing state-of-the-art topics of singularity, instability and unboundedness manifesting in finite times in differential equations towards new foundations of these complex and rich characteristics.

**Organizer(s) :** Kaname Matsue

**Classification :** 34D05, 34M35, 35B44, 37C60, 70F16, Blow-up in ODEs and asymptotic expansions of solutions,<sup>[1]</sup> Blow-up in parabolic and hyperbolic PDEs,<sup>[2]</sup> Collision in celestial mechanics,<sup>[3]</sup> Monodromy matrices for ODEs in complex domain,<sup>[4]</sup> nonautonomous instability in ODEs and PDEs

**Minisymposium Program :**

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00988 (1/2) : 1C @G402 [Chair: Kaname Matsue]

## [01480] Finite-time singularity and dynamics at infinity: characterization and asymptotic expansions

**Format :** Talk at Waseda University

**Author(s) :** Kaname Matsue (Kyushu University)

**Abstract :** Finite-time singularities in differential equations, in particular finite-time blow-up, from the viewpoint of dynamical systems are discussed in this talk.

Using compactifications of phase spaces and time-scale desingularization naturally introduced by the quasi-homogeneity of vector fields in an asymptotic sense, blow-up characterization is reduced to dynamics at infinity.

We also discuss a systematic calculations of multi-order asymptotic expansion of blow-up solutions with a natural correspondence to dynamical properties of invariant sets at infinity.

## [01461] Compactification for Asymptotically Autonomous Dynamical Systems with Applications to Tipping Points.

**Format :** Talk at Waseda University

**Author(s) :** Sebastian Wieczorek (University College Cork) Christopher K.R.T. Jones (University of North Carolina)

**Abstract :** We develop a general compactification framework for non-autonomous ODEs, where non-autonomous terms decay asymptotically. The aim is to use compact invariant sets of the autonomous limit systems from infinity to analyse non-autonomous instabilities in the original problem, in the spirit of dynamical systems theory. We illustrate our framework using rate-induced tipping instability that occurs in natural systems when external inputs, such as climatic conditions, vary faster than some critical rate.

## [01512] Rate-induced tipping in heterogeneous reaction-diffusion systems

**Format :** Talk at Waseda University

**Author(s) :** Cris Hasan (University of Glasgow) Sebastian Wieczorek (University College Cork) Ruaidhri Mac Cárthaigh (University College Cork)

**Abstract :** We propose a framework to study nonlinear waves in reaction-diffusion equations (RDEs) based on a compactification technique and Lin's method for constructing heteroclinic orbits. We identify generic instabilities of travelling pulses in an RDE with a fold of heteroclinic orbits in the compactified system. In an illustrative model of a habitat patch that is geographically shrinking or shifting due to climate change, we combine our framework with numerical continuation to study tipping points to extinction.

## [01527] Using Geometric Singular Perturbation Theory to Understand Singular Shocks

**Format :** Talk at Waseda University

**Author(s) :** Barbara Lee Keyfitz (The Ohio State University)

**Abstract :** Solutions to hyperbolic conservation laws (quasilinear hyperbolic partial differential equations) typically satisfy the equations in the sense of distributions. But there are examples of systems whose solutions have even lower regularity, solutions known as singular shocks or delta shocks. In some of these examples, candidates for solutions that exhibit singular shocks have been found as limits of approximations.

An unusual model in two-component chromatography, discovered by Marco Mazzotti, provides the first physically significant example of a system where singular shocks appear. This model does not fit into the existing theory.

Here, I present new approach. Singular perturbation theory (SPT), long a mainstay of classical applied mathematics, has been put on a new footing by an approach developed by Fenichel in the 1970's and since then extended by many other researchers. This approach uses manifold and dynamical systems theory to replace the formal constructions of SPT. It was first applied to singular shocks by Stephen Schecter. Using geometric singular perturbation theory, Ting-Hao Hsu, Martin Krupa, Charis Tsikkou and I can give a singular shock structure to Mazzotti's unusual chromatography equations.

00988 (2/2) : 1D @G402 [Chair: Kaname Matsue]

## [01810] Traveling wave solutions for certain 1D degenerate parabolic equation

**Format :** Talk at Waseda University

**Author(s) :** Yu Ichida (Meiji University)

**Abstract :** In this talk, the speaker will report results on the classification of the traveling wave solutions of the 1D degenerate parabolic equation and porous medium equation, and give observations and suggestions on phenomena corresponding to bifurcations of equilibria at infinity. These are obtained through dynamical systems theory and Poincar'e compactification. This talk includes a collaborative work with Professor Takashi Sakamoto at Meiji University.

## [02005] Blow-up Rates for Solutions of a Quasi-Linear Parabolic Equation

**Format :** Talk at Waseda University

**Author(s) :** Koichi Anada (Waseda University) Tetsuya Ishiwata (Shibaura Institute of Technology) Takeo Ushijima (Tokyo University of Science)

**Abstract :** The motion of curves by the power of their curvatures with positive exponent has been studied. The motion is described by a parabolic equation and some solutions blow up with Type II singularity. In this talk, we discuss the blow-up rates of solutions with Type II singularity. Precisely, we derive an asymptotic expansion of the traveling wave which plays a significant role and then we provide an upper estimate for the blow-up rates.

## [02492] Computation of collision and near-collision orbits in Celestial Mechanics problems.

**Format :** Talk at Waseda University

**Author(s) :** Shane Kepley (Vrije Universiteit) Jason Desmond Mireles James (Florida Atlantic University) Maciej Capinski (AGH University of Science and Technology)

**Abstract :**

Understanding connecting and collision/ejection orbits is central to the study of transport in Celestial Mechanics.

Finding and validating connecting orbits can be difficult in general, and is complicated even more by the presence of ejection/collisions which are singularities of the flow. We present a rigorous Levi-Cevita regularization algorithm which, combined with existing analytic continuation techniques, allows us to overcome this obstruction. This regularization is performed dynamically allowing invariant manifolds to be parameterized dynamically and globally, even near singularities.

## [04119] Rigorous numerics for finding the monodromy of Picard-Fuchs differential equations for a family of K3 toric hypersurfaces

**Format :** Talk at Waseda University

**Author(s) :** Akitoshi Takayasu (University of Tsukuba)Toshimasa Ishige (Chiba University)

**Abstract :** In this talk, we present a method for finding monodromy matrices of linear differential equations with finite-dimensional solution spaces via rigorous numerics. We also provide a computational result that gives monodromy matrices, which represent the fundamental group of the differential equation, of Picard-Fuchs differential equations for a certain family of K3 toric hypersurfaces.

## [00989] Structure and dynamics in complex biological systems

**Session Time & Room :**

00989 (1/2) : 2C (Aug.22, 13:20-15:00) @D515

00989 (2/2) : 2D (Aug.22, 15:30-17:10) @D515

**Type :** Proposal of Minisymposium

**Abstract :** Biological systems have been identified as complex networks consisting of many biomolecules and interactions between them. The dynamics of molecular activities based on such networks are considered to be the origin of biological functions. In the recent progress of mathematical sciences, various methods have been developed to determine important aspects of dynamical properties based on network topologies. Such theories may become breakthroughs to solve the dynamics of complex biological systems. In this symposium, we introduce a wide variety of topological approaches and discuss their future perspectives from both mathematical and biological points of view.

**Organizer(s) :** Takashi Okada, Yuji Hirono, Atsushi Mochizuki

**Classification :** 92Cxx, 93Bxx, 34Hxx

**Minisymposium Program :**

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00989 (1/2) : 2C @D515 [Chair: Takashi Okada]

## [01956] Controlling cell fate specification system based on network structure

**Format :** Talk at Waseda University

**Author(s) :** Atsushi Mochizuki (Institute for Life and Medical Sciences, Kyoto University)Kenji Kobayashi (Department of Zoology, Graduate School of Science, Kyoto University)Kazuki Maeda (Faculty of Informatics, The University of Fukuchiyama)Miki Tokuoka (Department of Zoology, Graduate School of Science, Kyoto University)Yutaka Satou (Department of Zoology, Graduate School of Science, Kyoto University)

**Abstract :** Modern biology provided large networks describing regulatory interactions between biomolecules. We developed Linkage Logic theory, which ensures observability and controllability of any long-term dynamics of the whole system by a subset of nodes, that is identified from the network alone as a feedback vertex set (FVS). We applied the theory to gene network for cell-fate specification in ascidian, including 92 genes. By manipulating 6 genes in FVS, all the seven tissues could be induced experimentally.

## [01938] An extension of the Fiedler-Mochizuki theory to time-delay systems

**Format :** Talk at Waseda University

**Author(s) :** Atsushi Kondo (Department of Mathematics, Kyoto University)

**Abstract :** We consider the dynamics of a system of differential equations called a Regulatory Network, which represents complex regulatory relationships such as gene regulatory networks. The paper by Fiedler-Mochizuki et al. (JDDE 2013) showed that it is possible to identify a set of determining nodes that determines the asymptotic dynamics of the Regulatory Network from its network structure alone. We extend this theory to the case where the regulatory network contains time delays.

## [01727] Structure-based and dynamics-based control of biological network models

**Format :** Talk at Waseda University

**Author(s) :** Jorge Gomez Tejeda Zanudo (Harvard Medical School)Reka Albert (Pennsylvania State University)Eli Newby (Pennsylvania State University)

**Abstract :** A task of interest when analyzing mathematical models of intracellular networks is to identify nodes that can provide attractor control in these systems. I will introduce stable motif control and feedback vertex set (FVS) control, two methods we have used to provide control strategies in multiple systems. I will discuss how we used FVS control and structure-based metrics based on signal propagation to identify high-ranking manipulations involving only 1-3 nodes that can provide attractor control.

## [01991] Universal structural requirements for maximal robust perfect-adaptation in biomolecular networks

**Format :** Talk at Waseda University

**Author(s) :** Ankit Gupta (ETH Zürich)Mustafa Khammash (ETH Zürich)

**Abstract :** Living systems survive in unpredictable environments by maintaining key physiological variables at their desired levels through tight regulation. This property is called robust perfect adaptation (RPA) and the aim of this talk is to mathematically characterize the structural requirements for biomolecular networks to attain a form of maximal RPA, whereby the network is simultaneously robust to the largest set of disturbances. These results provide a new Internal Model Principle for biomolecular RPA networks.

00989 (2/2) : 2D @D515 [Chair: Atsushi Mochizuki]

## [01961] Network topology determines robustness and flexibility in chemical reaction systems

**Format :** Talk at Waseda University

**Author(s) :** TAKASHI OKADA (Kyoto Univ)

**Abstract :** In living cells, biochemical reactions form complex networks. Conventional sensitivity analysis is limited by the need for detailed reaction kinetics and parameters, which are often not available for living systems. Our new method, structural sensitivity analysis, determines qualitative sensitivity solely from network structures. Based on this framework, we established a topological theorem that determines the extent to which the perturbation of a parameter affects chemical concentrations and fluxes within the network.

## [01937] Simplifying complex chemical reaction networks

**Format :** Talk at Waseda University

**Author(s) :** Yuji Hirono (Asia Pacific Center for Theoretical Physics)

**Abstract :** Understanding the behavior of complex biochemical reaction networks is an important and challenging problem. To ease the analysis, it is desirable if we can simplify a complex reaction network while preserving its important features. In this talk, we discuss a method for the reduction of chemical reaction networks. We identify topological conditions on its subnetworks, reduction of which preserves the original steady state exactly.

## [01907] Multistationarity conditions for polynomial systems in biology

**Format :** Talk at Waseda University

**Author(s) :** Carsten Conradi (HTW Berlin)

**Abstract :** Polynomial Ordinary Differential Equations are an important tool in quantitative biology. Often parameters vary in large intervals. Consequently one is interested in parameter conditions that guarantee multistationarity and further constrain parameter values. The focus of this talk are mass action ODEs that admit a monomial parameterization of positive steady states. For such systems it is straightforward to derive a parameterization of rate constants where multistationarity exists. Multisite phosphorylation systems are of this type.

## [02165] Global Attractor Conjecture, Persistence Conjecture, and Toric Differential Inclusions

**Format :** Talk at Waseda University

**Author(s) :** Gheorghe Craciun (University of Wisconsin-Madison)

**Abstract :** The Global Attractor Conjecture can be regarded as a far-reaching generalization of Boltzmann's H-theorem for finite dimensional systems. The related Persistence Conjecture is even more general, and essentially says that solutions of weakly reversible systems cannot go extinct. We will discuss some of these connections, and we focus especially on introducing Toric Differential Inclusions as a tool for proving these conjectures. We also describe implications for biochemical mechanisms for noise filtering and cellular homeostasis.

## [00994] Mathematical modeling approach in pharmacokinetics/pharmacodynamics

**Session Time & Room :** 1D (Aug.21, 15:30-17:10) @D515

**Type :** Proposal of Minisymposium

**Abstract :** Pharmacokinetics/pharmacodynamics (PK/PD) modeling is an essential component of drug discovery and development. PK modeling describes the relationship between dose and drug concentration while PD modeling quantifies the relationship between drug concentration and therapeutic effects. A model-based simulation could provide a scientific decision-making information in new drug development process and the prediction power for the success of clinical trial. The session is dedicated to discuss recent advances and challenges in PK/PD modeling and simulation to overcome fundamental limitation and conventional approaches.

**Organizer(s) :** Soyoung Kim, Seongwon Lee

**Classification :** 92C45

**Minisymposium Program :**

00994 (1/1) : 1D @D515 [Chair: Soyoung Kim]

## [05562] Principles and applications of clinical pharmacology and pharmacometrics in the drug development

**Format :** Talk at Waseda University

**Author(s) :** Sungpil Han (The Catholic University of Korea)

**Abstract :** In the rapidly evolving landscape of pharmaceutical research, clinical pharmacology and pharmacometrics have emerged as pivotal disciplines in the drug development process. This presentation will delve into the principles and applications of these disciplines, particularly focusing on the integration of mathematical modeling in pharmacokinetics/pharmacodynamics (PK/PD) to accelerate and optimize drug development.

Clinical pharmacology plays a crucial role in understanding the effects of a drug and the mechanisms of its actions in humans, while pharmacometrics aids in quantifying drug, disease, and trial information to aid efficient drug development and regulatory decisions. This presentation will discuss the synergy between these two disciplines, highlighting how they can form the bedrock for creating more effective, safer drugs.

A key element in this context is the employment of mathematical models in PK/PD studies. The presentation will demonstrate the use of such models to predict the time course of drug concentration and its consequent effects, thereby guiding optimal dosage and timing strategies. Special emphasis will be placed on the role of mathematical modeling in minimizing adverse drug reactions and predicting drug-drug interactions.

## [05550] Pharmacokinetic Model of Tacrolimus based on Stochastic Simulation and Estimation in Korean Adult Transplant Recipients

**Format :** Talk at Waseda University

**Author(s) :** Suein Choi (Catholic university of Korea)Seunghoon Han (Catholic university of Korea)

**Abstract :** Therapeutic drug monitoring (TDM) is a crucial clinical procedure that involves measuring drug concentrations in a patient's blood or other biological fluids to ensure optimal dosing. To achieve targeted exposure and improve dosing precision, the Bayesian estimation method is utilized, which optimizes individual pharmacokinetic (PK) parameters based on previous TDM data and a population PK model. The development of an accurate PK model is essential, as it integrates clinically relevant covariates and appropriate random effect parameters.

However, the nature of TDM data poses certain limitations for PK model development. Although it provides a wealth of real-world data reflecting a wide range of covariates, it primarily consists of trough concentrations, which restricts the information available for model building. To overcome these limitations, we employed the stochastic simulation and estimation (SSE) method, enabling the integration of published PK models with acquired real-world TDM data, even in the absence of raw data from the published models. This approach also allowed us to evaluate clinically meaningful covariates.

Using the SSE method, we successfully developed a population PK model for tacrolimus that encompasses both published PK models and newly collected TDM data from the Korean population. This model serves as a robust framework for practical TDM procedures, as it incorporates clinically relevant covariates and reflects real-world settings. Despite the inherent limitations associated with TDM data, the SSE method proved invaluable in leveraging the information contained within TDM data by integrating published PK models while accounting for model variability.

Overall, the developed population PK model for tacrolimus, utilizing the SSE method, represents a significant advancement in TDM practices. It enhances dosing precision, incorporates relevant covariates, and provides a solid foundation for guiding therapeutic strategies in clinical settings. By addressing the challenges posed by TDM data limitations, this research contributes to the refinement and optimization of pharmacokinetic modeling for improved patient outcomes.

## [01369] Distributional approaches expressing tumor delay of the transit compartment model

**Format :** Talk at Waseda University

**Author(s) :** Jong Hyuk Byun (Pusan National University)Il Hyo Jung (Pusan National University)

**Abstract :** Transit compartment model describes the way in which drugs inhibit the growth of tumors, based on a system of ODEs describing damaged cells' transition under the influence of the drug, using Erlang distribution. In our approach, Coxian distribution is used to model the various delays when the number of delay compartments is fixed. In the other approach, the delay compartments are combined into a single form using Mittag-Leffler distribution, without pre-specifying the number of compartments.

## [01975] Accurate Prediction of Drug Interactions Through Cytochrome P450 Induction

**Format :** Talk at Waseda University

**Author(s) :** Yun Min Song (KAIST)Ngoc-Anh Thi Vu (Chungnam National University)Quyen Thi Tran (Chungnam National University)Hwi-yeol Yun (Chungnam National University)Jung-woo Chae (Chungnam National University)Sang Kyum Kim (Chungnam National University)Jae Kyoung Kim (KAIST)

**Abstract :** FDA guidance has recommended several model-based predictions to determine potential drug-drug interactions (DDIs). In particular, the ratio of substrate AUCs under and not under the effect of enzyme inducers is predicted by the Michaelis-Menten model, which is valid only in low-enzyme-concentration conditions. We found that such DDI predictions lead to severe errors. To resolve this, we derived a new equation that significantly improves clinical DDI prediction, which is critical to preventing drug toxicity and failure.

# [01000] Advances in random dynamical systems and ergodic theory

## Session Time & Room :

01000 (1/3) : 2D (Aug.22, 15:30-17:10) @F309

01000 (2/3) : 2E (Aug.22, 17:40-19:20) @F309

01000 (3/3) : 3C (Aug.23, 13:20-15:00) @F309

**Type :** Proposal of Minisymposium

**Abstract :** Random or non-autonomous dynamical systems provide useful and flexible models to investigate systems whose evolution depends on external factors, such as noise or seasonal forcing. In recent years, there have been significant advances in the ergodic-theoretic investigation of random dynamical systems, allowing for an enhanced understanding of statistical properties, coherent structures, and the complicated interplay between noise and chaotic dynamics. This minisymposium presents the work of experts and emerging mathematicians working in this vibrant and evolving field, featuring both general-audience lectures giving an overview of the field, and expert-level talks on cutting-edge advances.

**Organizer(s) :** Alex Blumenthal, Cecilia Gonzalez-Tokman

**Classification :** 37H05, 37H15, 37H20, 37A50, 37C83

## Minisymposium Program :

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01000 (1/3) : 2D @F309 [Chair: Alex Blumenthal]

# [01338] Random dynamical systems and multiplicative ergodic theorems

**Format :** Talk at Waseda University

**Author(s) :** Cecilia Gonzalez Tokman (University of Queensland)

**Abstract :** Random dynamical systems are flexible mathematical models for the study of complicated systems whose evolution is affected by external factors, such as seasonal cycles and random effects. This talk will start with a broad introduction to the area, with an emphasis on multiplicative ergodic theory. Then, we will review recent advances in the field, which provide fundamental information for the study of transport phenomena in such systems.

# [05504] Compound Poisson Statistics for Random Dynamical Systems via Spectral Perturbation

**Format :** Talk at Waseda University

**Author(s) :** Jason Ath念 (University of Queensland)Gary Froyland (UNSW Sydney)Cecilia Gonzalez Tokman (University of Queensland)Sandro Vaienti (Aix Marseille Universite)

**Abstract :** In this talk we discuss recent results concerning the return time statistics for deterministic and random dynamical systems. Taking a perturbative approach, we consider a decreasing sequence of holes in phase space which shrink to a point. For systems satisfying a spectral gap, we show that limiting distribution of return times to these shrinking holes is a compound Poisson distribution. We provide specific examples of classes of transformations for which the limiting distribution is Polya-Aeppli.

# [01905] Entropy and pressure formulas for conditioned random dynamical systems

**Format :** Talk at Waseda University

**Author(s) :** Maximilian Engel (Free University of Berlin)Tobias Hurth (Free University of Berlin)

**Abstract :** Building upon recent results on Lyapunov exponents for memoryless random dynamical systems with absorption --- see Castro et al. 2022 ---, we establish the notion of metric entropy for this setting. We further discuss the relation between entropy, positive Lyapunov exponents and escape rates for such conditioned RDS, where the main example concerns the local dynamics of stochastic differential equations on bounded domains with escape through the boundary. This is joint work with Tobias Hurth.

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01000 (2/3) : 2E @F309 [Chair: Cecilia Gonzalez Tokman]

part\_2

## [01767] Lyapunov exponents for random perturbations of coupled standard maps

**Format :** Talk at Waseda University

**Author(s) :** Alex Blumenthal (Georgia Tech)Jinxin Xue (Tsinghua University)Yun Yang (Virginia Tech)

**Abstract :** In this talk, we show how to give a quantitative estimate for the sum of the first N Lyapunov exponents for random perturbations of a natural class  $2N$ -dimensional volume-preserving systems exhibiting strong hyperbolicity on a large but non invariant subset of phase space. Concrete models covered by our setting include systems of coupled standard maps, in both weak' and strong' coupling regimes. This is a joint work with Alex Blumenthal and Yun Yang.

## [05620] Shear-induced effects Random Dynamical Systems

**Format :** Talk at Waseda University

**Author(s) :** Dennis Chermann (Freie Universität Berlin)Maximilian Engel (Freie Universität Berlin)

**Abstract :** The mechanism of shear-induced chaos was first demonstrated by Wang and Young for periodic orbits perturbed by deterministic periodic kicking. In this talk I will present recent results on shear-induced chaos, as well as shear-induced blow-up, in random dynamical systems generated by stochastic differential equations with additive noise.

## [02045] Horseshoes for a class of non-uniformly expanding random circle maps

**Format :** Online Talk on Zoom

**Author(s) :** Giuseppe Tenaglia (Imperial College London)

**Abstract :** We prove the abundance of horseshoe-like behavior in random circle endomorphisms with a positive Lyapunov exponent under large IID noise conditions. By satisfying a transitivity requirement towards an expanding full branch and effectively controlling the tails of hyperbolic times, our results prove that any two disjoint intervals almost surely exhibit horseshoe-like behavior with full probability.

01000 (3/3) : 3C @F309 [Chair: Maximilian Engel]

## [05540] Continuation of attractors of random dynamical systems with bounded noise

**Format :** Talk at Waseda University

**Author(s) :** Jeroen Lamb (Imperial College London)Martin Rasmussen (Imperial College London)Konstantinos Kourliouros (Imperial College London)Dmitry Turaev (Imperial College London)Wei Hao Tey (IRCN, The University of Tokyo)Kalle Timperi (Oulu University)

**Abstract :** We study the problem of persistence of minimal invariant sets with smooth boundary for a class of discrete-time set-valued dynamical systems, naturally arising in the context of random dynamical systems with bounded noise. In particular, we introduce a single-valued map, the so-called boundary map, which has the property that a certain class of invariant submanifolds for this map is in one-to-one correspondence with invariant sets for the corresponding set-valued map. We show that minimal invariant sets with smooth boundary persist under small perturbations of the set-valued map, provided that the associated boundary map is normally hyperbolic at the unit normal bundle of the boundary.

## [05055] Noise-induced chaos and conditioned Lyapunov exponents in a random logistic map

**Format :** Talk at Waseda University

**Author(s) :** Bernat Bassols Cornudella (Imperial College London)Jeroen SW Lamb (Imperial College London)

**Abstract :** We consider a random logistic map with bounded additive noise, in the parameter regime where the deterministic logistic map has a stable period three cycle. We demonstrate how the transition from noise-induced synchronisation (negative Lyapunov exponent) to noise-induced chaos (positive Lyapunov exponent), arising as a result of growing noise amplitude, can be understood through a two-compartment approximation, effectively modelling the competition between contracting and expanding behaviour. Relevant characteristic exit times and conditioned Lyapunov exponents for the predominantly contracting and expanding compartments are obtained through quasi-stationary and quasi-ergodic invariant measures.

## [01453] On the quasi-ergodicity of absorbing Markov chains with unbounded transition densities, including random logistic maps with escape

**Format :** Online Talk on Zoom

**Author(s) :** Matheus Manzatto de Castro (Imperial College London) Jeroen S. W. Lamb (Imperial College London) Martin Rasmussen (Imperial College London) Vincent P. H. Goverse (Imperial College London)

**Abstract :** In this paper, we consider absorbing Markov chains  $X_n$  admitting a quasi-stationary measure  $\mu$  on  $M$  where the transition kernel  $\mathcal{P}$  admits an eigenfunction  $0 \leq \eta \in L^1(M, \mu)$ . We find conditions on the transition densities of  $\mathcal{P}$  with respect to  $\mu$ , which ensure that  $\eta(x)\mu(dx)$  is a quasi-ergodic measure for  $X_n$  and that the Yaglom limit converges to the quasi-stationary measure  $\mu$ -almost surely. We apply this result to the random logistic map  $X_{n+1} = \omega_n X_n(1 - X_n)$  absorbed at  $\$\\mathrm{R}\\setminus$

**[0,1], where  $\omega_n$  is an i. i. d sequence of random variables uniformly distributed in  $[a,b]$ , for  $1 \\leq a < 4$  and  $b > 4$ .**

## [01003] Mathematical Modeling and Simulation in Land-Ocean Transition Zones

**Session Time & Room :**

01003 (1/3) : 4E (Aug.24, 17:40-19:20) @D402

01003 (2/3) : 5B (Aug.25, 10:40-12:20) @D402

01003 (3/3) : 5C (Aug.25, 13:20-15:00) @D402

**Type :** Proposal of Minisymposium

**Abstract :** Around 30% of global populations live in coastal zones, which are facing increasing threats from both land and ocean. These include saltwater intrusion, storm surge, ecosystem degeneration and coastal erosion, to name a few. Mathematical modeling and simulation on multiple processes in the land-ocean transition zones are essential to understand intrinsic mechanisms and make reliable predictions for the future. This symposium aims to exchange new advances on mathematical modeling, numerical simulation, operational applications, and other relevant topics in hydrodynamic, ecological, and other processes in the land-ocean transition zones, thus to promote interdisciplinary collaborations in applied mathematics and earth science.

**Organizer(s) :** Dong Ye, Hui Wu, Hairong Yuan, Shengfeng Zhu

**Classification :** 76-10, 86A05, 76D55, 76D05, 74F10

**Minisymposium Program :**

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01003 (1/3) : 4E @D402

## [05505] Analytical solution to the elliptic PDE of shelf wave with the relaxation of semi-geostrophic approximation

**Format :** Talk at Waseda University

**Author(s) :** Hui Wu (East China Normal University)

**Abstract :** The response of a wide shelf to sub-inertial and barotropic offshore pressure signals from the shelf edge was investigated. By relaxing the semi-geostrophic approximation, an elliptical wave structure equation was formulated and solved with the integral transform method. It was found that when the imposed offshore signal has an along-shelf length scale similar to the shelf width, it can efficiently break the potential vorticity barrier and propagate towards the coast, producing a significant coastal sea-level set-up. Thereafter, the pressure signal reflects from the coast or the sloping topography, producing a transient eddy and propagates to the downshelf. The intensities of the coastal set-up and the eddy increase as the along-shelf scale of the sub-inertial signal decreases or when its timescale is close to the inertial period. For a signal with longer timescale, the eddy is insignificant. The

part\_2

nature of the shelf response is controlled by the shelf conductivity  $\kappa \equiv r((fsB))$ , in which  $r$  is the Rayleigh friction coefficient,  $f$  is the Coriolis parameter,  $s$  is the shelf slope, and  $B$  is the shelf width, respectively. For a given offshore signal, coastal set-up increases with  $\kappa$ . For large  $\kappa$ , the eddy energy is concentrated at low modes, producing a large eddy, whereas a small  $\kappa$  produces a small eddy. The proposed theory can explain coastal sea-level fluctuations under eddy impingement in the Mid-Atlantic Bight or other similar areas.

## [05568] Boundary layer dynamics of wave-current flows over cylindrical canopies

**Format :** Talk at Waseda University

**Author(s) :** Jun Ao Kan (Shanghai Jiao Tong University)Rui Wang (Shanghai Jiao Tong University)Hui Xu (Shanghai Jiao Tong University)

**Abstract :** Interactions of waves and currents with large roughness elements in the coastal ocean play a crucial role in drag generation and energy dissipation, which are quite different from the extensively-investigated smooth wall boundary layer or small-scale roughness. In the framework of high-order spectral/hp element method, the present study focuses on the analysis of implicit large eddy simulations of the combined current-wave flows over arrays of staggered circular cylinders with a diameter and a height of 0.5D. Unlike previous studies, our research examines array units that go beyond individual obstacles, enabling us to explore a wider range of physical mechanisms in turbulence, which consequently increases the computational complexity. By manipulating the wave amplitude, three distinct scenarios were obtained (i.e. pure current, weak wave and strong wave conditions, respectively) to analyze the effects of waves on currents or vice versa. The primary objective of current work is to investigate the energy transport mechanisms between the canopy and non-canopy layers, as well as the characteristics of the population of coherent structures. The dependences of energy budget, large-scale structures, sweeps and ejections are analyzed in detail.

## [05325] On discrete shape gradients of boundary type for PDE-constrained shape optimizations

**Format :** Talk at Waseda University

**Author(s) :** Wei Gong (Academy of Mathematics and Systems Science, Chinese Academy of Sciences)

**Abstract :** Shape gradients have been widely used in numerical shape gradient descent algorithms for shape optimization. The two types of shape gradients, i.e., the distributed one and the boundary type, are equivalent at the continuous level but exhibit different numerical behaviors after finite element discretization. To be more specific, the boundary type shape gradient is more popular in practice due to its concise formulation and convenience in combining with shape optimization algorithms but has lower numerical accuracy. In this talk we provide a simple yet useful boundary correction for the normal derivatives of the state and adjoint equations, motivated by their continuous variational forms, to increase the accuracy and possible effectiveness of the boundary shape gradient in PDE-constrained shape optimization. We consider particularly the state equation with Dirichlet boundary conditions and provide a preliminary error estimate for the correction. Numerical results show that the corrected boundary type shape gradient has comparable accuracy to that of the distributed one. Extensions to other type of PDE-constrained shape optimizations are also considered, including the interface identification problems, the eigenvalue problems, the Stokes and Navier-Stokes problems. Moreover, we give a theoretical explanation for the comparable numerical accuracy of the boundary type shape gradient with that of the distributed shape gradient for Neumann boundary value problems.

## [05596] An incremental SVD method for integro-differential equations: addressing storage and computational challenges

**Format :** Online Talk on Zoom

**Author(s) :** Yangwen Zhang (University of Louisiana at Lafayette)Gang Chen (Sichuan University)

**Abstract :** At the current stage, it is widely recognized that the numerical solution of integro-differential equations with a memory term depends on all previous time instances. Consequently, the storage requirement increases linearly, while the computational complexity grows quadratically with the number of time steps. This presents a significant challenge for numerical simulations, and to the best of our knowledge, it remains an unresolved issue. In this paper, we present a memory-free algorithm, based on the incremental SVD technique, that exhibits only linear growth in computational complexity as the number of time steps increases. Rigorous error analysis and numerical experiments will be presented to validate our approach.

## [05546] Causal AI Ocean Learning and Prediction

**Author(s)** : X. San Liang (Fudan University)

**Abstract** : Ocean-atmosphere forecasting is faced with many challenges such as open boundary condition specification, unresolved process parameterization, unknown physics modeling, etc. Even if all these are fixed, a more challenging issue that ever exists is the unpredictability intrinsically embedded in chaotic systems. The recent fast development of AI seems to be promising for a partial solution to these problems. But AI is also faced with the problem of interpretability. Due to the black-box nature, it is difficult for one to decide whether a forecast is acceptable or not. In this presentation, I will show how interpretability will be enhanced for AI algorithms with the aid of a recently developed causality analysis which has been rigorously established from first principles during the past 18 years (e.g., Liang, Information flow and causality as rigorous physical notions ab initio. Phys Rev E 94:052201, 2016). In the oceanographic context, this is easily understood as the tracing of predictability sources to make the maximal usage of information. Also the quantitative nature of the causality analysis allows for an adjustment of the neural network to remove spurious correlations toward an optimal performance. Demonstrated here will be an operational forecast of the surface circulation of a region in the South China Sea, and a decadal forecast of the Central Pacific-type El Niño.

## [02217] Parameterizing the baroclinic instability with an artificial potential energy term

**Format** : Online Talk on Zoom

**Author(s)** : Qingshan Chen (Clemson University)

**Abstract** : In a numerical model that is under-resolved in the horizontal and/or vertical directions, baroclinic instability is often suppressed, leading to a build-up of layer interface slopes and potential energy that can not be released. In this work, we demonstrate, within the multilayer shallow water model and the Hamiltonian framework, how the baroclinic instability can be parameterized by adding an artificial potential energy term based on the slope of the interior layer interfaces.

## [05534] Two-grid Finite Element Decoupling Scheme for the Mixed Navier-Stokes/Darcy Model

**Author(s)** : Yanren Hou (Xi'an Jiaotong University)

**Abstract** : For the mixed steady-state Navier-Stokes/Darcy model with BJS interface condition, a two-grid FEM based decoupling scheme is analyzed in the talk. The well-posedness of the discrete system and its optimal error estimation are obtained.

01003 (3/3) : 5C @D402

## [05525] Shape Optimization of Incompressible Navier-Stokes flows with Shape Gradients

**Format** : Talk at Waseda University

**Author(s)** : Shengfeng Zhu (East China Normal University)Jiajie Li (East China Normal University)

**Abstract** : Shape design of fluid flows has applications in engineering. We consider shape optimization of incompressible flows with shape gradients. Traditional boundary shape gradients have high smoothness requirement on the boundary and is less general than the distributed shape gradient. We consider numerically finite element approximations to the distributed and boundary corrected shape gradients. A prior error estimates are shown. Numerical results are reported to verify theory and show effectiveness of shape gradient algorithms.

## [03963] Simulation of Droplet-laden Turbulent Channel flow by LBM and Phase field method

**Format :** Online Talk on Zoom

**Author(s) :** Dingyi Pan (Zhejiang University)Yuqing Lin (Zhejiang University)

**Abstract :** Direct numerical simulation of droplet-laden turbulent channel flow is studied by coupled lattice Boltzmann method and phase field modeling with Cahn-Hilliard (CH) equation. The weighted essentially non-oscillatory (WENO) scheme is applied for the discretization of CH equation. The simulated friction Reynolds number is up to 180, and the mass conservation of droplet phase is well fulfilled. The results show that the existence of droplets contribute to the drag reduction of the turbulent channel flow.

## [01011] Analysis and Design of Dynamical Circuits, Systems and Networks

**Session Time & Room :** 5D (Aug.25, 15:30-17:10) @A207

**Type :** Proposal of Minisymposium

**Abstract :** In order to properly design electric circuits and other dynamical systems and networks, it is important to understand their structures and dynamics through mathematical analysis. This minisymposium brings together four engineering researchers working on dynamical circuits, systems and networks to present their recent research results on analysis and design from various perspectives such as discrete harmonic analysis, bifurcation analysis, model order reduction, mathematical programming and contraction mapping principle, with applications to metamaterials, communications, control and signal processing. Through their talks, the importance of mathematics in engineering will be demonstrated.

**Organizer(s) :** Norikazu Takahashi

**Classification :** 94Cxx, 94Dxx, 34Hxx, 65Kxx, 90Cxx

**Minisymposium Program :**

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01011 (1/1) : 5D @A207 [Chair: Norikazu Takahashi]

## [01717] Network dynamics on electric circuits and Maxwell's equations

**Format :** Talk at Waseda University

**Author(s) :** Takashi Hisakado (Kyoto University)

**Abstract :** Electric circuits are the network dynamics of voltages and currents, and electromagnetic phenomena described by Maxwell's equations can be appropriately modeled and designed on the network. In the presentation, we will summarize the properties of electric circuits as discrete harmonic analysis and show that by considering the relationship between Maxwell's equations and electric circuits, a new type of electric circuit can be used to design metamaterials, antennas, etc.

## [01871] Design of a delayed feedback controller based on bifurcation analysis

**Format :** Talk at Waseda University

**Author(s) :** Koki Yoshida (National Institute of Technology, Toyama College)Keiji Konishi (Osaka Metropolitan University)Naoyuki Hara (Osaka Metropolitan University)

**Abstract :** In addition to stabilizing an operating point, increasing the basin size is required to construct a robust system against disturbances. However, the time delays in the system or control dynamics make it difficult to estimate the basin size analytically. This presentation will show how to design a delayed feedback controller that expands the basin size of the operating point in a DC bus system with the help of a numerical bifurcation analysis tool.

## [02715] Nonlinear Model Order Reduction for CT Image Reconstruction

**Format :** Talk at Waseda University

**Author(s) :** Yuichi Tanji (Kagawa University)Ken'ichi Fujimoto (Kagawa University)

**Abstract :** X-ray computed tomography apparatus is widely used in clinics to determine whether there is a tumor inside the human body. In this study, we present how to generate a prediction model for image reconstruction using nonlinear model order reduction of the nonlinear dynamical system. For the model reduction, we use proper orthogonal decomposition. We improve the computational techniques so that many observed data can be considered, which provides effective orthogonal vectors for model reduction.

## [02712] Analysis and Design of Recurrent Neural Networks Generating Desired Sequences of Bipolar Vectors

**Format :** Talk at Waseda University

**Author(s) :** Norikazu Takahashi (Okayama University)Tsuyoshi Yamakawa (Kyushu University)Yasuhiro Minetoma (Kyushu University)Tetsuo Nishi (Kyushu University)Tsuyoshi Migita (Okayama University)

**Abstract :** Recurrent neural networks or RNNs can generate a variety of pattern sequences by the time evolution of each neuron's output. We derive sufficient conditions under which an RNN described by a system of piecewise linear differential equations can generate a desired pattern sequence, and present mathematical programming problems to find its parameter values that satisfy those conditions. Furthermore, we analyze the convergence of state trajectories of an RNN to a limit cycle using a fixed-point theorem and the contraction mapping principle.

# [01024] Multiscale modeling and simulation methods of inhomogeneity in defected systems

**Session Time & Room :**

01024 (1/3) : 3E (Aug.23, 17:40-19:20) @D102

01024 (2/3) : 4C (Aug.24, 13:20-15:00) @D102

01024 (3/3) : 4D (Aug.24, 15:30-17:10) @D102

**Type :** Proposal of Minisymposium

**Abstract :** Inhomogeneity, as the source of various multiscale effects in systems such as materials and data, play essential roles in the material properties and the data structure of these defected systems with multiple scales. The complexity of modeling defects and their impact to the properties of the systems present new challenges for mathematical modeling and analysis. Multi-scale, multi-physics and multi-fidelity models are required to accurately describe the complicated phenomena associated with the inhomogeneity. Speakers in this minisymposium will discuss recent advances in modeling approaches and simulation methods, and new findings obtained in analysis and simulations.

**Organizer(s) :** Shuyang Dai, Luchan Zhang

**Classification :** 74-10

**Minisymposium Program :**

01024 (1/3) : 3E @D102 [Chair: Luchan Zhang]

## [04025] Recent progress on multiscale coupling for crystalline defects

**Format :** Talk at Waseda University

**Author(s) :** Lei Zhang (Shanghai Jiao Tong University)Yangshuai Wang (University of British Columbia)

**Abstract :** In this talk, we present some recent progress on the multiscale coupling methods for crystalline defects, which include: 1) MeshAC, a three-dimensional mesh package designed for atomistic-to-continuum; 2) (a/c) coupling with higher order far-field boundary conditions; 3) Adaptive QM/MM coupling with machine-learned interatomic potentials (MLIP).

part\_2

## [02228] Mathematical perspectives in modeling microstructures in metallic materials

**Format :** Online Talk on Zoom

**Author(s) :** Yejun Gu (Agency for Science Technology and Research)

**Abstract :** The mechanical properties of metallic materials are strongly dependent on their microstructural features (e.g. morphology and distribution of dislocations, grains, and other defects). Thus it necessitates a comprehensive understanding of the microstructure evolutions in materials during deformation. I will present some attempts of applying mathematical methods to address this problem. The presentation consists of two parts: one is the fast algorithms for solving partial differential equations, in order to precisely describe the microstructure evolutions; the other is the probabilistic description and statistical analysis, which are employed to quantify the relationship between the microstructures and mechanical properties.

## [04547] A Three-Dimensional Continuum Simulation Method for Grain Boundary Motion Incorporating Dislocation Structure

**Format :** Talk at Waseda University

**Author(s) :** Xiaoxue Qin (Shanghai University)

**Abstract :** We develop a continuum model for the dynamics of grain boundaries in three dimensions that incorporates the motion and reaction of the constituent dislocations. The continuum model is based on a simple representation of densities of curved dislocations on the grain boundary. Illposedness due to nonconvexity of the total energy is fixed by a numerical treatment based on a projection method that maintains the connectivity of the constituent dislocations. An efficient simulation method is developed, in which the critical but computationally expensive long-range interaction of dislocations is replaced by another projection formulation that maintains the constraint of equilibrium of the dislocation structure described by the Frank's formula. This continuum model is able to describe the grain boundary motion and grain rotation due to both coupling and sliding effects, to which the classical motion by mean curvature model does not apply. Comparisons with atomistic simulation results show that our continuum model is able to give excellent predictions of evolutions of low angle grain boundaries and their dislocation structures.

## [04727] A nonlocal elasticity model for simulating the static and dynamic problems of crystalline defects in materials

**Format :** Talk at Waseda University

**Author(s) :** Xiaoyin Wang (Wuhan University)

**Abstract :** In this work, we present a nonlocal elasticity model in order to solve the static and dynamic problems related to crystalline defects such as dislocations, interfaces, etc. In our model, a superposition framework based on nonlocal description is used to solve the stress and displacement field due to defects. The interaction of dislocation with other types of defects such as cracks can be modeled with higher accuracy due to the consideration of nonlocal effects. The model is solved by optimization based numerical techniques in order to accelerate the simulations. We also apply this model to problems related to crystal interfaces.

01024 (2/3) : 4C @D102 [Chair: Shuyang Dai]

## [05384] An IVP of a model for motion of grain boundaries

**Format :** Talk at Waseda University

**Author(s) :** Peicheng Zhu (Shanghai University)

**Abstract :** We shall prove global existence of weak solutions to an initial-boundary value problem for a novel phase-field model which is proposed as an attempt to describe the motion of grain boundaries, a type of interface motion by interface diffusion driven by bulk free energy in elastically deformable solids. Its applications include important processes arising in Materials science, e.g., Sintering. In this model the evolution equation for an order parameter is a non-uniformly, degenerate parabolic equation of fourth order, which differs from the Cahn-Hilliard equation by a non-smooth term of the gradient of the unknown.

## [04942] Stochastic Continuum Models for High-Entropy Alloys with Short-range Order

**Format :** Talk at Waseda University

**Author(s) :** Luchan Zhang (Shenzhen University) Yahong Yang (Hong Kong University of Science and Technology) Yang Xiang (Hong Kong University of Science and Technology)

**Abstract :** High entropy alloys (HEAs) are a class of novel materials that exhibit superb engineering properties. It has been demonstrated by extensive experiments and first principles/atomistic simulations that short-range order in the atomic level randomness strongly influences the properties of HEAs. In this talk, we present stochastic continuum models for HEAs with short-range order from atomistic models. A proper continuum limit is obtained such that the mean and variance of the atomic level randomness together with the short-range order described by a characteristic length are kept in the process from the atomistic interaction model to the continuum equation. The obtained continuum model with short range order is in the form of an Ornstein–Uhlenbeck (OU) process, which validates our previous continuum model adopting the OU process phenomenologically for HEAs with short range order. We derive such stochastic continuum models with short-range order for both elasticity in HEAs without defects and HEAs with dislocations (line defects). The obtained stochastic continuum models are based on the energy formulations, whose variations lead to stochastic partial differential equations.

## [03918] GAS: A Gaussian Mixture Distribution-Based Adaptive Sampling Method for PINNs

**Format :** Talk at Waseda University

**Author(s) :** Cheng Yuan (Wuhan University)

**Abstract :** With the recent study of deep learning in scientific computation, the Physics-Informed Neural Networks (PINNs) method has drawn widespread attention for solving Partial Differential Equations (PDEs). Compared to traditional methods, PINNs can efficiently handle high-dimensional problems, but the accuracy is relatively low, especially for highly irregular problems. Inspired by the idea of adaptive finite element methods and incremental learning, we propose GAS, a Gaussian mixture distribution-based adaptive sampling method for PINNs. During the training procedure, GAS uses the current residual information to generate a Gaussian mixture distribution for the sampling of additional points, which are then trained together with historical data to speed up the convergence of the loss and achieve higher accuracy. Several numerical simulations on 2D and 10D problems show that GAS is a promising method that achieves state-of-the-art accuracy among deep solvers, while being comparable with traditional numerical solvers.

## [05016] An Elastic Interaction-Based Loss Function in Image Segmentation and Detection

**Format :** Talk at Waseda University

**Author(s) :** Yixin FENG (Hong Kong University of Science and Technology) Yuan Lan (Huawei Theory Lab) Yang Xiang (Hong Kong University of Science and Technology) Luchan Zhang (Shenzhen University)

**Abstract :** Deep learning techniques have shown their success in image processing since they are easy to manipulate and robust to various types of datasets. The commonly used pixel-wise loss functions result in a bottleneck to achieve high precision for complicated structures in biomedical and autonomous driving science images. For example, the predicted small blood vessels in retinal images are often disconnected or even missed under the supervision of the pixel-wise losses, and the existence of lanes needed to be inferred even when they are occluded by cars or human. This long-range elastic interaction-based training strategy addresses these problem. In this strategy, convolutional neural network (CNN) learns the target region under the guidance of the elastic interaction energy between the boundary of the predicted region and that of the actual object. Under the supervision of the proposed loss, the boundary of the predicted region is attracted strongly by the object boundary and tends to stay connected.

01024 (3/3) : 4D @D102 [Chair: Luchan Zhang]

## [03366] Phase field model for self-climb of prismatic dislocation loops by vacancy pipe diffusion

**Format :** Online Talk on Zoom

**Author(s) :** Xiaohua NIU (Xiamen University of Technology)

**Abstract :** In this talk, we present a phase field model for the self-climb motion of prismatic dislocation loops via vacancy pipe diffusion driven by elastic interactions. This conserved dynamics model is developed under the

framework of the Cahn-Hilliard equation with incorporation of the climb force on dislocations, and is based on the dislocation self-climb velocity formulation established in Ref. (Niu et al., 2017). Asymptotic analysis shows that the proposed phase field model gives the dislocation self-climb velocity accurately in the sharp interface limit. Numerical simulations of evolution, translation, coalescence and repelling of prismatic loops by self-climb show excellent agreement with discrete dislocation dynamics simulation results and the experimental observation. Also a phase field model for the motion of prismatic dislocation loops by both conservative climb and non-conservative climb is also developed. The simulations will be shown to illustrate the influence of the self-climb in the dislocation climb process.

## [05129] Global weak solutions to an initial-boundary value problem of a phase-field model for motion of grain boundaries

**Author(s)** : Luchan Zhang (Shenzhen University)Peicheng Zhu (Shanghai University)

**Abstract** : We shall prove global existence of weak solutions to an initial-boundary value problem for a novel phase-field model which is proposed as an attempt to describe the motion of grain boundaries, a type of interface motion by interface diffusion driven by bulk free energy in elastically deformable solids. Its applications include important processes arising in Materials science, e.g., Sintering. In this model the evolution equation for an order parameter is a non-uniformly, degenerate parabolic equation of fourth order, which differs from the Cahn-Hilliard equation by a non-smooth term of the gradient of the unknown.

## [01028] High-order numerical methods for nonlinear PDEs

**Session Time & Room :**

01028 (1/3) : 2E (Aug.22, 17:40-19:20) @E708

01028 (2/3) : 3C (Aug.23, 13:20-15:00) @E708

01028 (3/3) : 3D (Aug.23, 15:30-17:10) @E708

**Type** : Proposal of Minisymposium

**Abstract** : Nonlinear partial differential equations (PDEs) have been widely used in various fields, such as thermodynamics, biology, material science, electromagnetism, to name just a few. Even though the history of the study on numerical PDEs is quite long, there are still many open and important questions. In this mini-symposium, we aim at gathering researchers working on the topic to discuss recent advances on the development and numerical analysis of high-order numerical methods for approximately solving nonlinear PDEs, in order to further promote the developments of the topic.

**Organizer(s)** : Buyang Li, Weifeng Qiu, Zhi Zhou

**Classification** : 65Mxx, 65Nxx, 65Bxx

**Minisymposium Program :**

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01028 (1/3) : 2E @E708 [Chair: Buyang Li]

## [05134] Error Analysis of IMEX and Time-Splitting Schemes for the Logarithmic Schrodinger's Equation

**Author(s)** : Li-Lian Wang (Division of Mathematical Sciences, Nanyang Technological University)

**Abstract** : The Schrodinger's equation with a logarithmic nonlinear term (LogSE):  $f(u)=u \log(|u|^2)$  exhibits rich dynamics, but such a nonlinearity presents significant challenges in both numerical solution and error analysis. Compared with usual cubic case,  $f(u)$  is non-differentiable at  $u=0$  but possesses certain Holder continuity. In this talk, we shall report our recent attempts in numerical study of LogSE with a focus on time discretization via implicit-explicit scheme and time-splitting scheme and on the introduction of new tools for the error analysis. This talk is based on joint works with Jingye Yan (Jiangsu University, China) and Xiaolong Zhang (Hunan Normal University, China).

## [02750] Constructing structure-preserving schemes via Lagrange multiplier approach

**Author(s)** : Qing Cheng (Tongji University)Jie Shen (Purdue University)

**Abstract** : In the talk, I will introduce a new Lagrange multiplier approach to construct efficient and accurate structure-preserving schemes for a class of semi-linear and quasi-linear parabolic equations. To be more specific, I will introduce how to construct positivity/bound-preserving, length-preserving, energy-dissipative schemes for a large class of PDEs. I will establish stability results under a general setting, and carry out an error analysis for second-order structure-preserving schemes. Finally, I will apply our approach to several typical PDEs which preserve structures described above. Some numerical results will be presented to validate our approach.

## [04415] Optimal $L^2$ error estimates of unconditionally stable FE schemes for the Cahn-Hilliard-Navier-Stokes system

**Author(s)** : Wentao Cai (Beijing Computational Science Research Center)Weiwei Sun (BNU-HKBU United International College)Jilu Wang (Harbin Institute of Technology (Shenzhen))Zongze Yang (The Hong Kong Polytechnic University)

**Abstract** : The paper is concerned with the analysis of a popular convex-splitting finite element method for the Cahn-Hilliard-Navier-Stokes system, which has been widely used in practice. Since the method is based on a combined approximation to multiple variables involved in the system, the approximation to one of the variables may seriously affect the accuracy for others. Optimal-order error analysis for such combined approximations is challenging. The previous works failed to present optimal error analysis in  $L^2$ -norm due to the weakness of the traditional approach. Here we first present an optimal error estimate in  $L^2$ -norm for the convex-splitting FEMs. We also show that optimal error estimates in the traditional (interpolation) sense may not always hold for all components in the coupled system due to the nature of the pollution/influence from lower-order approximations. Our analysis is based on two newly introduced elliptic quasi-projections and the superconvergence of negative norm estimates for the corresponding projection errors. Numerical examples are also presented to illustrate our theoretical results. More important is that our approach can be extended to many other FEMs and other strongly coupled phase field models to obtain optimal error estimates.

01028 (2/3) : 3C @E708 [Chair: Zhi Zhou]

## [05392] Pointwise-in-time a posteriori error control for higher-order discretizations of time-fractional parabolic equations

**Author(s)** : Natalia Kopteva Sebastian Franz (Technical University Dresden)

**Abstract** : Time-fractional parabolic equations with a Caputo time derivative are considered. For such equations, we explore and further develop the new methodology of the a-posteriori error estimation and adaptive time stepping proposed in [N. Kopteva, Pointwise-in-time a posteriori error control for time-fractional parabolic equations, Appl. Math. Lett., 123 (2022)]. We improve the earlier time stepping algorithm based on this theory, and specifically address its stable and efficient implementation in the context of high-order methods. The considered methods include an L1-2 method and continuous collocation methods of arbitrary order, for which adaptive temporal meshes are shown to yield optimal convergence rates in the presence of solution singularities.

## [05204] An $L^1$ mixed DG method for second-order Elliptic Equations in the Non-divergence Form

**Author(s)** : Weifeng Qiu (City University of Hong Kong)Jin Ren (Old Dominion University)Ke Shi (Old Dominion University)Yuesheng Xu (Old Dominion University)

**Abstract** : In this talk we present an  $L^1$  mixed DG method for second-order elliptic equations in the non-divergence form. The elliptic PDE in nondivergence form arises in the linearization of fully nonlinear PDEs. Due to the nature of the equations, classical finite element methods based on variational forms can not be employed directly. In this work, we propose a new optimization based finite element method which combines the classical DG framework with recently developed  $L^1$  optimization technique. Convergence analysis in both energy norm and  $L^\infty$  norm are obtained under weak regularity assumption of the PDE ( $H^1$ ). Such  $L^1$  optimization problems are nondifferentiable and invalidate traditional gaidnet methods. To overcome this difficulty, we characterize solutions of  $L^1$  optimization as fixed-points of proximity equations and utilize matrix splitting technique to obtain a class of fixed-point proximity algorithms with convergence analysis. In addition, various numerical examples will be displayed to validate the analysis in the end.

## [02310] New analysis of a mixed FEM for Ginzburg-Landau Equations

**Author(s)** : Huadong Gao (Huazhong University of Science and Technology)

**Abstract** : This talk is concerned with new error analysis of a lowest-order backward Euler Galerkin-mixed finite element method for the time-dependent Ginzburg-Landau equations. The method is based on a commonly-used non-uniform approximations ( $P_1, ND_1 \times RT_0$ ), which has been widely used. We establish the second-order accuracy for the order parameter in spatial direction, although the accuracy for  $(\text{curl}\mathbf{A}, \mathbf{A})$  is in the first order only. Our numerical experiments confirm the optimal convergence of  $\psi_h$ .

## [01989] Spectral analysis of a mixed method for linear elasticity

**Author(s)** : Xiang Zhong (City University of Hong Kong)Weifeng Qiu (City University of Hong Kong)

**Abstract** : We consider a mixed method for linear elasticity eigenvalue problem, which approximates numerically the stress, displacement, and rotation, by piecewise  $(k+1)$ ,  $k$  and  $(k+1)$ -th degree polynomials ( $k \geq 1$ ) on Hsieh-Clough-Toucher grids. The numerical eigenfunction of stress is symmetric. By the discrete  $H^1$ -stability of numerical displacement, we prove an  $O(h^{k+2})$  approximation to the  $L^2$ -orthogonal projection of the eigenspace of exact displacement for the eigenvalue problem, with proper regularity assumption. We also prove that numerical approximation to the eigenfunction of stress is locking free with respect to Poisson ratio. We introduce a hybridization to reduce the mixed method to a condensed eigenproblem and prove an  $O(h^2)$  initial approximation of the eigenvalue by using the discrete  $H^1$ -stability of numerical displacement.

01028 (3/3) : 3D @E708 [Chair: Zhi Zhou]

## [05520] A convergent algorithm for the interaction of mean curvature flow and surface diffusion

**Author(s)** : Charles M. Elliott (University of Warwick)Harald Garcke (University of Regensburg)Balázs Kovács (Paderborn University)

**Abstract** : In this talk we will discuss a numerical approach for the interaction of mean curvature flow and a diffusion process on the surface.

The evolving surface finite element discretisation is analysed for a coupled geometric PDE system.

We will present an algorithm based on a system coupling the diffusion equation to evolution equations for geometric quantities in the velocity law for the surface; give insight into the stability estimates; which lead to optimal-order  $H^1$ -norm error estimates.

We will present numerical experiments reporting on: convergence, preservation of mean convexity, loss of convexity, weak maximum principles, and the occurrence of self-intersections.

Based on a joint work with C. M. Elliott (Warwick) and H. Garcke (Regensburg).

## [02942] Optimal convergence of the arbitrary Lagrangian-Eulerian second-order projection method for the Navier-Stokes equations on an evolving domain

**Author(s)** : Buyang Li (The Hong Kong Polytechnic University)Qiqi Rao (The Hong Kong Polytechnic University)Yupei Xie (The Hong Kong Polytechnic University)

**Abstract** : In this talk, we introduce how to prove the optimal convergence of the arbitrary Lagrangian-Eulerian second-order projection method for the Navier-Stokes equations on an evolving domain.

## [03545] Exponential Spectral Method for Semilinear Subdiffusion Equations with Rough Data

**Author(s)** : Qiqi RAO (PolyU)

**Abstract** : A new spectral method is constructed for the linear and semilinear subdiffusion equations with possibly discontinuous rough initial data. The new method effectively combines several computational techniques, including the contour integral representation of the solutions, the quadrature approximation of contour integrals, the exponential integrator using the de la Vallée Poussin means of the source function, and a decomposition of the time interval geometrically refined towards the singularity of the solution and the source function. Rigorous error analysis shows that the proposed method has spectral convergence for the linear and semilinear subdiffusion

equations with bounded measurable initial data and possibly singular source functions under the natural regularity of the solutions.

## [01029] Extremal Combinatorics and Probabilistic Combinatorics

### **Session Time & Room :**

01029 (1/3) : 4C (Aug.24, 13:20-15:00) @G304

01029 (2/3) : 4D (Aug.24, 15:30-17:10) @G304

01029 (3/3) : 4E (Aug.24, 17:40-19:20) @G304

**Type :** Proposal of Minisymposium

**Abstract :** Combinatorics studies discrete objects and their properties, which has striking applications in statistical physics, biology, computer science and so on. This minisymposium we propose will focus on Extremal Combinatorics and Probabilistic Combinatorics, which are two of the most central branches of modern combinatorial theory. We aim to attract the top researchers to the minisymposium, where they will present their recent results, discuss open problems, exchange research ideas, and initiate new collaborations. We expect the minisymposium will have a lasting impact in this area.

**Organizer(s) :** Guanghui Wang, Shenggui Zhang

**Classification :** 05Dxx

### **Minisymposium Program :**

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01029 (1/3) : 4C @G304

## [03243] Turan problem for graphs from geometric shapes

**Format :** Talk at Waseda University

**Author(s) :** Hong Liu (Institute for Basic Science)

**Abstract :** While Tur'án type problem is the most studied topic in extremal combinatorics, some of the most basic bipartite degenerate Tur'án problems remain elusive. In this talk, I will discuss some recent advancements on this topic and new results on bipartite graphs arising from geometric shapes and periodic tilings commonly found in nature, including even prisms, planar hexagonal tiling and quadrangulations of plane, cylinder and torus. This is joint work with Jun Gao, Oliver Janzer, Zixiang Xu.

## [03233] Robust linear algebra methods and some applications

**Format :** Talk at Waseda University

**Author(s) :** Jun Gao (Institute for Basic Science)Hong Liu (Institute for Basic Science)Zixiang Xu (Institute for Basic Science)

**Abstract :** Given a set  $L \subseteq [n]$ , what can we say about the size or structure of a set system  $\mathcal{F} \subseteq 2^{[n]}$  if  $A \star B \in L$  for  $A, B \in \mathcal{F}$ , where  $\star \in \{\cap, \cup, \setminus, \triangle\}$ . Many important results have been produced around the above questions, and several far-reaching methods have been developed. In this talk, I will explain how to apply the linear algebra methods in the above problems, and introduce an algebraic proof of the stability result for Kleitman's theorem.

## [03332] Optimal bisections of directed graphs

**Format :** Talk at Waseda University

**Author(s) :** Guanwu Liu (University of Science and Technology of China)Jie Ma (University of Science and Technology of China)Chunlei Zu (Shanghai Jiaotong University)

**Abstract :** In this paper, motivated by a problem of Scott and a conjecture of Lee, Loh and Sudakov we consider bisections of directed graphs. We prove that every directed graph with  $m$  arcs and minimum semidegree at least  $d$  admits a bisection in which at least  $\left(\frac{d}{2(2d+1)} + o(1)\right)m$  arcs cross in each direction. This provides an optimal bound as well as a positive answer to a question of Hou and Wu in a stronger form.

## [03231] Hypergraphs with infinitely many extremal constructions

**Format :** Online Talk on Zoom

**Author(s) :** JIANFENG HOU (Fuzhou University)

**Abstract :** We give the first exact and stability

results for a hypergraph Tur'{{a}n problem with infinitely many extremal constructions that are far from each other in edit-distance.

This includes an example of triple systems with Tur'{{a}n density 2/9, thus answering some questions posed by the third and fourth authors and Reiher about the feasible region of hypergraphs. Our results also provide extremal constructions whose shadow density is a transcendental number.

Our novel approach is to construct certain multilinear polynomials that attain their maximum (in the standard simplex) on a line segment and then to use these polynomials to define an operation on hypergraphs that gives extremal constructions.

01029 (2/3) : 4D @G304

## [04610] Embeddings in “random like” hypergraphs

**Format :** Talk at Waseda University

**Author(s) :** Guanghui Wang (Shandong University)

**Abstract :** An archetype problem in extremal combinatorics is to study the structure of subgraphs appearing in different classes of (hyper)graphs. We will focus on such embedding problems in “random like” hypergraphs. In precise, we will mention Turan problems in quasi-random hypergraphs.

## [03333] Spectral extremal graphs for disjoint cliques

**Format :** Talk at Waseda University

**Author(s) :** Liying Kang (Shanghai University)

**Abstract :** Let  $kK_{r+1}$  be the graph consisting of  $k$  vertex-disjoint copies of the complete graph  $K_{r+1}$ .

Moon [Canad. J. Math. 20 (1968) 95–102] and Simonovits [Theory of Graphs (Proc. colloq., Tihany, 1996)] independently showed that if  $n$  is sufficiently large, then the join of a complete graph  $K_{k-1}$  and an  $r$ -partite Tur'{{a}n graph  $T_{n-k+1,r}$  is the unique extremal graph for  $kK_{r+1}$ . In this talk we consider the graph which has the maximum spectral radius among all graphs without  $k$  disjoint cliques. We show that if  $G$  attains the maximum spectral radius over all  $n$ -vertex  $kK_{r+1}$ -free graphs for sufficiently large  $n$ , then  $G$  is isomorphic to the join of a complete graph  $K_{k-1}$  and an  $r$ -partite Tur'{{a}n graph  $T_{n-k+1,r}$ . This is a joint work with Zhenyu Ni, Jing wang.

## [03579] Co-degree threshold for rainbow perfect matchings in uniform hypergraphs

**Format :** Talk at Waseda University

**Author(s) :** Hongliang Lu (Xi'an Jiaotong University)Yan Wang (Shanghai Jiao Tong University)Xingxing Yu (Georgia Institute of Technology)

**Abstract :** Let  $k$  and  $n$  be two integers, with  $k \geq 3$ ,  $n \equiv 0 \pmod{k}$ , and  $n$  sufficiently large. We determine the  $(k-1)$ -degree threshold for the existence of a rainbow perfect matchings in  $n$ -vertex  $k$ -uniform hypergraph. This implies the result of R'odl, Ruci'nski, and Szemer'edi on the  $(k-1)$ -degree threshold for the existence of perfect matchings in  $n$ -vertex  $k$ -uniform hypergraphs. In our proof, we identify the extremal configurations of closeness, and consider whether or not the hypergraph is close to the extremal configuration. In addition, we also develop a novel absorbing device and generalize the absorbing lemma of R'odl, Ruci'nski, and Szemer'edi.

## [03715] Recent progress on non-separating subgraphs in highly connected graphs

**Format :** Talk at Waseda University

**Author(s) :** Shinya Fujita (Yokohama City University)

**Abstract :** Let  $k$  be a positive integer. A connected graph  $G$  is said to be  $k$ -connected, if for any vertex subset  $S$  of  $V(G)$  such that  $|S|$

01029 (3/3) : 4E @G304

## [04621] Spanning trees with bounded number of leaves in $K_{1,p}$ -free graphs

**Format :** Talk at Waseda University

**Author(s) :** Kenta Ozeki (Yokohama National University)

**Abstract :** Matthews and Sumner proved that a connected  $K_{1,3}$ -free graph contains a Hamiltonian path if the graph satisfies a certain minimum degree condition.

Extending this result, it has been widely studied about the existence of a spanning  $k$ -ended tree in  $K_{1,3}$ -free or  $K_{1,4}$ -free graphs with  $k \geq 2$ , and in  $K_{1,5}$ -free graphs with  $k = 4, 6$ , where a  $k$ -ended tree is a tree with at most  $k$  leaves. With this situation in mind, in this talk, we pose a conjecture on a spanning  $k$ -ended tree in  $K_{1,p}$ -free graphs, and show two partial answers to the conjecture:

One solves the case  $p = 5$  completely, and the other proves the conjecture asymptotically for all  $p \geq 6$ .

This is a joint work with Masao Tsugaki (Tokyo University of Science) and partially with Masahiro Kimura (Yokohama National University).

## [04636] Hadwiger's conjecture for some graphs with independence number two

**Format :** Talk at Waseda University

**Author(s) :** Guiying YAN (Academy of Mathematics and Systems Science'Chinese Academy of Sciences)Qiang Zhou (Academy of Mathematics and Systems Science'Chinese Academy of Sciences)

**Abstract :** Hadwiger's conjecture is difficult to prove even for graphs with independence number two. Recently, Daniel Carter

found the conjecture is true for  $H$ -free graphs if  $H$  is some particular graphs of 6, 7, 8 or 9 vertices with the help of computers. In this talk, we will introduce this conjecture is true if  $H$  is one of four special graphs with 6 or 7 vertices

mathematically.

## [05371] On Connectivities of Edge-Colored Graphs

**Format :** Talk at Waseda University

**Author(s) :** Kiyoshi Yoshimoto (Nihon University)

**Abstract :** In this talk, we consider two kind of color-connectivities of edge-colored graphs which are generalizing strong connectivity of directed graphs and also the relation is given.

Furthremore we show structures of edge-colored complete graphs using the color-connectivities.

# [01036] Progress in Mathematical Programming Methods and Applications

**Session Time & Room :**

01036 (1/2) : 3C (Aug.23, 13:20-15:00) @A208

01036 (2/2) : 3D (Aug.23, 15:30-17:10) @A208

**Type :** Proposal of Industrial Minisymposium

**Abstract :** (Mixed-)integer (non-)linear optimization has been one of the biggest successes in transferring mathematical insight into real-world impact. Due to the generality of the integer programming model combined with continuous improvement in solving capability, the list of industrial applications is virtually endless. While the problems are usually NP-hard in theory, in practice, an incredible number of real-world instances can be solved within seconds. The algorithmic progress outpaced the increase in computer performance by far; combined, the solver speed has exponentially grown over the last 40 years. We present the latest state-of-the-art and a glimpse into the future.

**Organizer(s) :** Thorsten Koch, Yuji Shinano

**Classification :** 90C90, 90C11, 68R05, 90-04

**Minisymposium Program :**

01036 (1/2) : 3C @A208 [Chair: Yuji Shinano]

## [05521] An efficient solver for multi-objective onshore wind farm siting and network integration

**Author(s)** : Thorsten Koch (Technische Universität Berlin / Zuse Institute Berlin)Jaap Pedersen (Zuse Institute Berlin)

**Abstract** : Existing planning approaches for onshore wind farm siting and network integration often do not meet minimum cost solutions or social and environmental considerations. In this talk, we present an approach for the multi-objective optimization of turbine locations and their network connection using the Quota Steiner tree problem. We design an exact solver that makes large problem instances solvable and outperforms generic MIP solvers. Although our case studies in selected regions of Germany show large trade-offs between the objective criteria of cost and landscape impact, small burdens on one criterion can significantly improve the other. In addition, we demonstrate that contrary to many approaches for exclusive turbine siting, network integration must be simultaneously optimized in order to avoid excessive costs or landscape impacts in the course of a wind farm project. Our novel problem formulation and the developed solver can assist planners in decision making and help optimize wind farms in large regions in the future.

## [02270] Steepest-Edge Simplex Algorithms for Quadratic Programming

**Format** : Talk at Waseda University

**Author(s)** : Shoji Shimizu (NTT DATA Mathematical Systems Inc.)Koichi Fujii (NTT DATA Mathematical Systems Inc.)Julian Hall (University of Edinburgh)

**Abstract** : We present steepest-edge simplex algorithms for quadratic programming problems. It is well known that in linear programming problems, the steepest-edge rule or Devex rule greatly reduces the total number of iterations in the simplex method. We extend these rules to the simplex method for quadratic programming and show their effectiveness through numerical experiments.

## [02259] Techniques and advances for solving MINLPs

**Author(s)** : Robert Luce (Gurobi)

**Abstract** : We consider solving mixed-integer nonlinear optimization problems to global optimality. Our solver is based on the common branch-and-bound paradigm, but includes a number of specialized techniques to deal with nonconvex constraints and nonconvex objective functions. In this talk we will outline a few of these components from a theoretical and computational point of view.

## [02296] New MIP presolving techniques in the Cardinal Optimizer

**Format** : Online Talk on Zoom

**Author(s)** : Gerald Gamrath (COPT GmbH)

**Abstract** : Presolving is an essential component of modern MIP solvers. Besides model cleanup, it identifies structures in the problem and tightens the formulation before the branch-and-cut search starts. In this talk, we discuss common structures in real-world instances and show how a mathematical analysis of those structures resulted in new presolving reductions implemented in the Cardinal Optimizer (COPT). The impact of the new techniques is demonstrated in computational experiments.

01036 (2/2) : 3D @A208 [Chair: Thorsten Koch]

## [05523] News from the FICO Xpress MIP Solver and Global MINLP Solver

**Author(s)** : Thorsten Koch (Technische Universität Berlin / Zuse Institute Berlin)Timo Berthold (Fair Isaac Germany GmbH)

**Abstract** : We will present the latest algorithmic advances and new features of the FICO Xpress Solver family. Next to enhanced MIP performance, a focus will be on recent new technologies like the ability to solve multi-objective optimization problems and mixed-integer nonlinear optimization problems to proven global optimality.

## [03882] Realization of smart factories using MIP

**Format** : Talk at Waseda University

**Author(s)** : Hiroki Ishikura (Kyushu University)

**Abstract** : Smart factories have become widely used for more efficient production activities recently. In collaboration with Rohto Pharmaceutical Co. (Rohto), we have conducted research to realize smart factories. In

part\_2

this talk, we will introduce mobility optimization related to automated warehouses. Rohto uses an automated warehouse to manage a large volume of various items. By optimizing the mobility of automated warehouses, production activities can be streamlined, and factory operations can be made more efficient.

## [02009] Benders' decomposition approach for the integrated long-haul and local VRP

**Format :** Talk at Waseda University

**Author(s) :** Junko Hosoda (Hitachi, Ltd.)Stephen J. Maher (Quantagonia GmbH)Yuji Shinano (Zuse Institute Berlin )Christoffer Villumsen (Hitachi, Ltd.)

**Abstract :** A supply chain management problem that integrates the determination of consolidation locations with the coordination of long-haul and local vehicle routing is a complicated problem. A Benders' decomposition approach is used to solve this problem. The delivery area and consolidation locations are computed in the master problem, and the long-haul and local vehicle routes are computed in the subproblems. The effectiveness of the decomposition is discussed in the presentation.

## [05524] Progress in Mathematical Programming Solvers from 2001 to 2020 and future Challenges

**Format :** Talk at Waseda University

**Author(s) :** Thorsten Koch (Technische Universität Berlin / Zuse Institute Berlin)

**Abstract :** We investigate the progress made in LP and MILP solver performance during the last two decades. On average, we found that for solving LP/MILP, the total speed-up was about 180 and 1,000 times, respectively. However, these numbers considerably underestimate the progress made on the algorithmic side: many problem instances can nowadays be solved within seconds, which the old codes are not able to solve within any reasonable time.

Finally, we will comment on future developments.

## [01037] From interacting particles to social dynamics: modelling and analysis of agent-based systems

**Session Time & Room :** 1E (Aug.21, 17:40-19:20) @G802

**Type :** Proposal of Minisymposium

**Abstract :** Modelling of social dynamics, including social media or epidemics, has a long tradition.

Recently, stochastic modelling has become more relevant, touching upon such diverse aspects as uncertainty quantification or robust control. Despite recent advances, there is still a gap between the theoretical analysis of models and the model calibration based on empirical data. In this minisymposium, we aim at bringing together researchers from dynamical systems, scientific computing and empirical research to discuss connections between agent-based models, particle systems and social simulation, with particular focus on the numerical analysis of agent-based models, reduced-order models and the role of random forcing.

**Organizer(s) :** Ana Djurdjevac, Carsten Hartmann

**Classification :** 35Qxx, 91Dxx, 37Hxx

**Minisymposium Program :**

01037 (1/1) : 1E @G802 [Chair: Ana Djurdjevac]

## [04502] Feedback loops in opinion dynamics of agent-based and mean-field models

**Format :** Talk at Waseda University

**Author(s) :** Natasa Conrad (Zuse Institute Berlin)Ana Djurdjevac (Freie Universität Berlin)Jonas Koepl (Weierstraß-Institut Berlin)

**Abstract :** We present a new mathematical model for co-evolving opinion and social dynamics within a group of part\_2

mobile, interacting agents. Agents' movements are governed by their social position and opinions of others, and opinion dynamics are affected by their proximity and opinion similarity. We investigate the behaviour of this ABM in different regimes, study the empirical distribution, and, in the limit of infinite number of agents, we derive a corresponding reduced model given by a PDE.

### [03486] Bounded Confidence Models of Opinion Dynamics

**Format :** Talk at Waseda University

**Author(s) :** Benjamin Goddard (University of Edinburgh) Grigoris Pavliotis (Imperial College London)

**Abstract :** Bounded confidence models postulate that people only take into account the opinions of others if they are already sufficiently close in 'opinion space' (i.e., they somewhat agree). I will introduce agent-based, ODE, SDE, and PDE models, before focusing on the (nonlocal, nonlinear) PDE case. The main results concern the complex dynamics that arise; the presence of 'phase transitions' under varying parameters; the importance of boundary conditions; and the introduction of 'radicals' with unchanging opinions.

### [04255] Open systems of interacting particles: a probabilistic and multiscale framework

**Format :** Talk at Waseda University

**Author(s) :** Mauricio del Razo (Freie Universität Berlin)

**Abstract :** Open systems are ubiquitous in nature and can be found in a variety of applications, such as chemical reactions, biological processes and even social dynamics. In this talk, we will introduce a comprehensive probabilistic framework for open systems of interacting particles. We will further discuss how our framework can be used to systematically construct consistent multiscale models and simulation schemes by examining how the framework scales up in different limiting regimes, such as system size and large population.

### [04762] Branching and coalescing particles in a singular environment

**Format :** Talk at Waseda University

**Author(s) :** Tommaso-Cornelis Rosati (University of Warwick)

**Abstract :** In this talk we analyse how the presence of a random, highly irregular, environment can influence the evolution of particle systems. We study the fluctuations of branching particles in a white-in-space environment, leading to a rough super-process. Further, we describe the scaling limit of a system of Brownian motions driven by a singular drift by means of the so-called Brownian castle. Joint works with N. Perkowski and (in progress) M. Hairer and G. Cannizzaro.

## [01040] Optimization and its Applications

**Session Time & Room :**

01040 (1/2) : 3D (Aug.23, 15:30-17:10) @F312

01040 (2/2) : 3E (Aug.23, 17:40-19:20) @F312

**Type :** Proposal of Minisymposium

**Abstract :** This minisymposium focuses on recent advances in mathematical optimization with versatile subjects such as optimal control, variational analysis, dynamical systems, nonlinear functional analysis, network systems, fixed point theory, and so forth. Application topics discussed here mainly lie in mathematical economics and engineering, in particular, optimal economic growth, general equilibrium analysis, utility theory, and Marxian economics as well as generative adversarial networks, but possible applications are not necessarily restricted to such problems. The minisymposium serves for a communication with applied mathematics in different areas.

**Organizer(s) :** Nobusumi Sagara, Alexander Zaslavski, Yuhki Hosoya

**Classification :** 49J27, 68M01, 91A27, 91B50, 91B62

**Minisymposium Program :**

01040 (1/2) : 3D @F312 [Chair: Yuhki Hosoya]

## [01444] Non-Smooth Integrability Theory

**Format :** Talk at Waseda University

**Author(s) :** Yuhki Hosoya (Chuo University)

**Abstract :** We study a method of calculating the utility function from a candidate of a demand function that is not differentiable but is locally Lipschitz. Using this method, we obtain two new necessary and sufficient conditions for a candidate of a demand function to be a demand function. The first is conditions for the Slutsky matrix, and the second is the existence of a concave solution to a partial differential equation. Moreover, we show that the upper semi-continuous weak order that corresponds to the demand function is unique, and this weak order is represented by our calculated utility function. We provide applications of these results to econometric theory. First, we show that, under several requirements, if a sequence of demand functions converges to some function with respect to the metric of compact convergence, then the limit is also a demand function. Second, the space of demand functions that have uniform Lipschitz constants on any compact set is complete under the above metric. Third, the mapping from a demand function to the calculated utility function becomes continuous. This implies that a consistent estimation method for the demand function immediately defines a consistent estimation method for the utility function using our calculation method.

## [01446] Theoretical analysis of two time-scale update rule for training GANs

**Format :** Talk at Waseda University

**Author(s) :** Naoki Sato Hideaki Iiduka (Meiji University)

**Abstract :** A theoretical analysis of a two time-scale update rule (TTUR) for training generative adversarial networks (GANs) has been given using decaying learning rates. In this talk, we give a theoretical analysis of TTUR using constant learning rates and show that, for TTUR using constant learning rates, the number of steps needed to train GAN decreases as the batch size increases. We also provide numerical results to support our theoretical analyses.

## [01450] Production Prices and Walrasian Intertemporal Competitive Equilibrium Prices in a Generalized Neoclassical Production Economy

**Format :** Talk at Waseda University

**Author(s) :** Naoki Yoshihara (University of Massachusetts Amherst)

**Abstract :** We examine a general correspondence between production prices in classical and Marxian economics and the Walrasian competitive equilibrium prices in the standard general equilibrium theory by considering a standard intertemporal economy with a discounted lifetime utility function and a set of general neo-classical production technologies. This work resembles Duménil and Levy (1985) and Dana et. al (1989), but unlike these, a path of intertemporal Walrasian equilibrium prices is characterized by the Euler equation, derived from the economic model in this paper. In addition, equilibrium factor prices are endogenously determined and can vary across periods. Therefore, our intertemporal Walrasian equilibrium is much closer to the standard neoclassical type, compared to the intertemporal competitive equilibrium defined by Dana et. al (1989). However, we will show that any intertemporal Walrasian equilibrium prices converge to a system of production prices in the long term.

## [01982] Optimal Growth in the Two-Sector Robinson-Shinkai-Leontief Model

**Format :** Talk at Waseda University

**Author(s) :** Minako Fujio (Yokohama National University)Ali M. Khan (The Johns Hopkins University)Liuchun Deng (Yale-NUS College)

**Abstract :** In this talk we synthesize the findings on the two-sector Robinson-Shinkai-Leontief model of optimal growth with and without discounting and demonstrate a variety of optimal dynamics. We provide a taxonomy of the optimal policy and the dynamics it yields for the entire parameter space of the model. At the same time, we shall focus on the two approaches we rely on to delineate those results, the value-loss minimization and the dynamic programming.

## [02153] On the approximate purification of mixed strategies in games with infinite action sets

**Format :** Talk at Waseda University

**Author(s) :** Chaowen Yu (Rissho University)Yuhki Hosoya (Chuo University)

**Abstract :** We consider a game in which the action set of each player is uncountable, and show that, from weak assumptions on the common prior, any mixed strategy has an approximately equivalent pure strategy. The assumption of this result can be further weakened if we consider the purification of a Nash equilibrium. Combined with the existence theorem for a Nash equilibrium, we derive an existence theorem for a pure strategy approximated Nash equilibrium under sufficiently weak assumptions. All of the pure strategies we derive in this paper can take a finite number of possible actions.

## [03646] Numerical aspects of finding nonlinear production – consumption equilibrium

**Format :** Talk at Waseda University

**Author(s) :** Igor Griva (George Mason University)Roman A Polyak (George Mason University)

**Abstract :** We present and analyze numerical results obtained by using extra pseudo-gradient (EPG) method on a set of randomly generated nonlinear production – consumption equilibrium (NPCE) problems. The obtained results show that the number of EPG steps required for finding NPCE grows linearly with the number of products of a given economy. The number of arithmetic operations or time required for finding NPCE grows as a cube of the number of products.

## [04476] Envelope theorems in Optimization

**Author(s) :** Joël Blot (Université PParis 1 Panthéon-SorbonneUniversi)

**Abstract :** We present recent results on the Envelope theorems in three chapters of Optimization. First in Static Optimization, secondly in Calculus of Variations and thirdly in Optimal Control Theory. To do that, we provide new results on the continuous dependence of coordinates in a moving frame, on the Hadamard differentiability of functionals under the integral form, and on the proof of the Pontryagin principle.

Date: November 13, 2022.

# [01043] Applications of applied mathematics towards ocean engineering and related technologies

**Session Time & Room :**

01043 (1/4) : 3C (Aug.23, 13:20-15:00) @G605

01043 (2/4) : 3D (Aug.23, 15:30-17:10) @G605

01043 (3/4) : 3E (Aug.23, 17:40-19:20) @G605

01043 (4/4) : 4C (Aug.24, 13:20-15:00) @G605

**Type :** Proposal of Industrial Minisymposium

**Abstract :** A reasonable knowledge about the response of nonlinear offshore dynamical systems under environmental loads is necessary but challenging. This is due to the coupling of internal forces along with external excitations. In this mini symposium, mathematical model of nonlinear offshore systems will be considered with the intention of keeping the response close to the desired one. This can be achieved using sub-optimal control mechanism derived from nonlinear quadratic regulator theory and also its associated data can be visualized via ensemble statistical sense.

**Organizer(s) :** Manikandan R, R.Sakthivel

**Classification :** 37C60

**Minisymposium Program :**

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01043 (1/4) : 3C @G605 [Chair: Prof. R.Sakthivel]

## **[01637] Robust control design for an autonomous underwater vehicle with uncertain dynamics**

**Format :** Online Talk on Zoom

**Author(s) :** Antony Crispin Sweety Charles Selvaraj (Avinashilingam Institute for Home Science and Higher Education for Women, Coimbatore)

**Abstract :** In this talk, we consider the robust control problem for autonomous underwater vehicles in the presence of nonlinearities and uncertainties. The aim is to obtain a robust controller in order to maneuver to any given point and track a moving target in the presence of parametric uncertainty and external disturbances. Specifically, the proposed state feedback robust controller guarantees the closed-loop system stability in the sense of the Lyapunov stability theory. Finally, simulation results are provided to verify the effectiveness of the control design.

## **[01719] Particle swarm optimization based robust controller for autonomous underwater vehicle**

**Format :** Online Talk on Zoom

**Author(s) :** Pankajavalli Palanisamy Balamani (Bharathiar University)Abinandhitha Radhakrishnan (Bharathiar University)

**Abstract :** The purpose of this work is to design a Particle Swarm Optimization (PSO) based controller in a systematic way to get the superior performance and robustness of the considered autonomous underwater vehicle model. Further, simulation results demonstrated the effectiveness of the proposed controller. The developed controller provides faster convergence to the change of parameters as compared to the conventional state feedback controller, for the stabilization of the closed-loop systems with external disturbances.

## **[01959] Applications of applied mathematics towards dynamic control of multi-dimensional structures**

**Format :** Online Talk on Zoom

**Author(s) :** Payel Chaudhuri (IIT KHARAGPUR)

**Abstract :** This work addresses an evolutionary optimal dynamic inversion algorithm-based semi-active controller for vibration reduction. The proposed inverse control algorithm is established on robust mathematical conceptualization and is ideal with semi-active magnetorheological dampers. The optimum voltage estimated from the proposed controller aid in generating the required control force from the MR dampers to the structures under dynamic loading. The resilience of the proposed inverse control algorithm is evaluated employing various seismic time histories on a multi-dimensional structure.

## **[01807] Ship maneuvering in waves**

**Format :** Talk at Waseda University

**Author(s) :** Rameesha T V (Scientist B)Krishnankutty P (Professor (Retired))

**Abstract :** Poor controllability of a surface ship is considered as a major cause for most of the marine accidents, which may result in loss of life and property. The present proposal is focused on the prediction of ship maneuvering in waves. Mathematical model for maneuvering prediction is modified for wave condition. The steering and turning characteristics of a container ship in still water and wave condition are compared experimentally and numerically.

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01043 (2/4) : 3D @G605 [Chair: Dr.Alankrita Singh]

## **[01761] AuX (X = Cu, Ag) monolayers promising Thermoelectric materials**

**Format :** Online Talk on Zoom

**Author(s) :** Kulwinder Kaur (Mehr Chand Mahajan DAV College for Women, Chandigarh)

**Abstract :** Under the application of strain, the electronic and thermoelectric properties of AuX (X = Cu, Ag) monolayers are investigated using density functional theory with the help of Boltzmann transport equations. At 6% strain, ultralow lattice thermal conductivity is observed. The maximum value of ZT is 2.20 and 1.40 for unstrained

part\_2

case and enhances to 3.61 and 2.91 at 6% strain for AuCu and AuAg monolayers, respectively, which compare favorably to several promising thermoelectric materials.

## [01770] One-Dimensional Hetero-Nanothread Fibres for high mechanical energy storage Applications

**Format :** Online Talk on Zoom

**Author(s) :** Marutheeswaran Srinivasan (Amrita Vishwa Vidyapeetham)Ramesh Sivasamy (Amrita Vishwa Vidyapeetham)

**Abstract :** Searching for high density energy materials is a key challenge for the engineering sciences. Recently discovered carbon nanothread bundles (CNB) exhibit higher mechanical strengths than carbon nanotube bundles. MD simulation and continuum elastic theory show that CNB exhibits a high mechanical energy storage density of up to 1.76 MJ kg<sup>-1</sup>. The results suggest CNB is an ideal candidate for fiber applications. We look at how mechanical behavior changes with heteroatom doping in the pristine state.

## [01763] The Li-based quaternary Heusler compound LiYPdSn: A promising thermoelectric material

**Format :** Online Talk on Zoom

**Author(s) :** Jaspal Singh Dhillon (Mata Sundri University Girls College)

**Abstract :** A newly discovered Li-based quaternary Heusler compound LiYPdSn is investigated which is the 18 Valence Electron Count (VEC) rule follower, non-magnetic, stabilized in FCC cubic structure of F-43m space group, possessing a melting point of 1700K. The Boltzmann transport equations and the Density Functional Theory is employed to investigate its dynamic stability, electronic band structure, thermodynamic response, motivating mechanical and elastic properties, thermodynamic response, which finally results in favorable thermoelectric performances and safe environmental opportunities.

## [02187] Mathematical modeling and Environmental Impact of COVID 19 pandemic

**Format :** Online Talk on Zoom

**Author(s) :** Satarupa Dey (Shyampur Siddheswari Mahavidyalaya)

**Abstract :** The corona virus disease was declared as a global pandemic on the year 2020 due to its rapid spread and complex impact on human health. By the end of the pandemic in 2021, there has been numerous impacts on environment. The prolonged lockdown enhanced the quality of air and water in urban areas on the other hand use of personal protective equipment and mask have increased plastic pollution in water bodies due to its improper disposal. In this study the positive as well as negative impact of corona virus pandemic on environment is discussed.

01043 (3/4) : 3E @G605 [Chair: Dr. Satarupa Dey]

## [01894] Highly Stable Lead-Free Magnetic Perovskite semiconductors

**Format :** Online Talk on Zoom

**Author(s) :** Shakeel Ahmad Khandy (Zhejiang University)

**Abstract :** Lead Free Halide Perovskites play a key role in Solar cell, LED, nondestructive bioimaging, long-wave communications, and medical care applications as they emit in the broader regions of spectrum from near-infrared region to visible range. Cs<sub>2</sub>MoX<sub>6</sub> (X=Cl,Br) as key members of the luminescent family, have been reported to emit light in ultraviolet and visible regions. Both these systems grow in cubic phase and are stable under thermal, mechanical and dynamical constraints of density functional theory. In addition, the ferromagnetic interactions of Mo with halide p-states create a total magnetic moment of 2 mB, thus enabling another degree of freedom to play with

## [02416] CFD of impingement over a curved surface by equilaterally staggered jets

**Format :** Online Talk on Zoom

**Author(s) :** Alankrita Singh (Indian Institute of Technology Roorkee)

**Abstract :** The equilateral staggered arrangement of jets constitutes of a central jet surrounded by four neighboring jets. The concave plate is uniformly heated at constant heat flux of 3 kW/m<sup>2</sup>. SIMPLE is incorporated

part\_2

for pressure velocity coupling. SST k- $\omega$  is used as the turbulence model. The solution is assumed to be converged when sum of the normalized residuals drop to e-5 for momentum, continuity and turbulence equations and e-7 for energy equations. Similar to lampblack visualization results, the CFD results show stretching of flow along the corners of the concave target surface.

## **[02634] An application of the Fuzzy inference system to Seismic Damage Prediction**

**Format :** Online Talk on Zoom

**Author(s) :** Dr. Champakali Das (Nims University)Dr. Narendra Kumar (Nims University)Dr. Amit Kumar Singh (RBS Engineering College)

**Abstract :** A damage prediction form has been developed by using fuzzy logic techniques. An earthquake caused significant damage to any building. The results of damage prediction must be used as the basis for a disaster preparedness plan if loss of life and property is to be reduced. Fuzzy logic offers a more unified strategy for addressing earthquake damage prediction difficulties because of the interconnectedness of the key components and the ambiguity of the ideas at play.

01043 (4/4) : 4C @G605 [Chair: Dr Payel Chaudhuri]

## **[03120] The Li-based quaternary Heusler compound LiYPdSn: A promising thermoelectric material**

**Format :** Online Talk on Zoom

**Author(s) :** Jaspal Singh Dhillon (Mata Sundri University Girls College)

**Abstract :** A newly discovered Li-based quaternary Heusler compound LiYPdSn is investigated which is the 18 Valence Electron Count (VEC) rule follower, non-magnetic, stabilized in FCC cubic structure of F-43m space group, possessing a melting point of 1700K. The Boltzmann transport equations and the Density Functional Theory is employed to investigate its dynamic stability, electronic band structure, thermodynamic response, motivating mechanical and elastic properties, thermodynamic response, which finally results in favorable thermoelectric performances and safe environmental opportunities.

## **[03204] Structural, electronic, dynamical and thermoelectric performance of LaCoTiSn Heusler alloy**

**Format :** Online Talk on Zoom

**Author(s) :** Yuhit Gupta (GSSS Badbar, Department of School Education, Punjab, India )

**Abstract :** In the present report, the physical properties of LaCoTiSn have been investigated by employing density functional theory. The calculated electronic band structure revealed the half-metallic character and 100% spin-polarization ratio suggest the ferromagnetic nature of the alloy. The evaluated value of Poisson's ratio '0.34' revealed the metallic bonding. To examine lattice dynamical stability, the phonon frequencies have been computed for first time. To measure the efficiency, the figure of merit is achieved to be 0.35.

## **[01050] Delay equations in mathematical biology**

**Session Time & Room :** 4E (Aug.24, 17:40-19:20) @G402

**Type :** Proposal of Minisymposium

**Abstract :** The mathematical modelling of many biological systems require the application of delay differential equations, since the future evolution of such systems depend of the duration of various processes. Examples range from cell cycle length in cell biology, maturation delay in population dynamics, and latency period in epidemiology. Time delays naturally occur in the control of biological systems as well. On the other hand, delay differential equations pose great challenges from the modelling, analysis, and numerical points of view, especially if nonlinearities are present and the delay is defined in a more involved way, such as state dependent delays. The goal of this minisymposium is to highlight recent advances and novel applications of delay equations in the field of mathematical biology.

**Organizer(s)** : Gergely Röst**Classification** : 34K05, 92-XX**Minisymposium Program** :

01050 (1/1) : 4E @G402 [Chair: Gergely Röst]

**[04514] An approach to model the bird migration****Format** : Talk at Waseda University**Author(s)** : Rongsong Liu (University of Wyoming)Stephen Gourley (Surrey University)**Abstract** : An approach to modelling bird migration is proposed, in which there is a region where birds do not move but spend time breeding. Birds leave this breeding region and enter a migration flyway. Mathematically, the flyway is a curve parametrised by arc-length. Per-capita mortality along the flyway is both position and age-dependent.**[05022] Infectious disease dynamics with delayed control on the reproduction number****Format** : Talk at Waseda University**Author(s)** : Ferenc A Bartha (Bolyai Institute, University of Szeged)**Abstract** : We attempt to mitigate an epidemic governed by a compartmental transmission model by introducing an adaptive control based on the effective reproduction number  $\mathcal{R}_t$ . The control aims to keep  $\mathcal{R}_t$  within the prescribed interval  $\mathcal{I}$  containing 1 by triggering or lifting non-pharmaceutical interventions affecting the transmission rate. The inherent delay in measuring the control output, i.e.  $\mathcal{R}_t$ , results in involved dynamics. We analyze the effects of both the choice of  $\mathcal{I}$  and of the delay.**[04371] A delayed epidemic model for behavior change****Format** : Talk at Waseda University**Author(s)** : Toshikazu Kuniya (Kobe University)**Abstract** : In the period of COVID-19, the on/off of strict interventions such as lockdown caused oscillations of reported infected population in many countries. In this study, we formulate a delayed epidemic model with psychological effect that people change their contact frequency according to the recent information on the reported cases. We perform the Hopf bifurcation analysis, and show that time delay and behavior change play an important role in the occurrence of the recurrent epidemic waves.**[04511] Evolution of maturation delay****Format** : Talk at Waseda University**Author(s)** : Gergely Röst (University of Szeged, Hungary)**Abstract** : We propose a new mathematical model to address the evolution of maturation period, building on the well-studied Nicholson's blowfly equation, formulated as a system of delay differential equations with two delays. We identify the optimal maturation delay, depending on the quality and suitability of the habitat, which is both a globally evolutionary stable and convergence stable strategy. Mathematically interesting questions raised by the invasibility of oscillatory insect populations. Joint work with Xingfu Zou.**[01054] Scalable Solvers for Multiphysics Problems****Session Time & Room** :

01054 (1/3) : 4D (Aug.24, 15:30-17:10) @E507

01054 (2/3) : 4E (Aug.24, 17:40-19:20) @E507

01054 (3/3) : 5B (Aug.25, 10:40-12:20) @E507

**Type :** Proposal of Minisymposium

**Abstract :** Many applications in computational sciences and engineering involve multiple physical quantities. Accurate simulations of multiphysics problems involve the solution of large sparse linear equation systems consisting of blocks that correspond to the different physics and their coupling. This has to be taken into account when designing scalable and efficient solvers for such kind of problems.

This minisymposium addresses the development and implementation of the solution strategies for large-scale complex multiphysics systems as well as the presentation of results on modern supercomputers.

**Organizer(s) :** Alexander Heinlein, Matthias Mayr

**Classification :** 65F08, 65F10, 65N55, 65N22

**Minisymposium Program :**

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01054 (1/3) : 4D @E507 [Chair: Alexander Heinlein]

## [01909] On the Use of Algebraic Multigrid in Various Applications on High Performance Computers

**Format :** Talk at Waseda University

**Author(s) :** Ulrike Meier Yang (Lawrence Livermore National Laboratory)

**Abstract :** The hypre software library provides a variety of parallel linear solvers implemented for high performance computers. Its focus is on algebraic multigrid methods (AMG), which provide excellent scalability. With the increasing inclusion of accelerators into current and future high-performance computers, various new programming models have been added to take advantage of the increased performance potential of GPUs. This talk will discuss porting challenges and present results of use of hypre's GPU-enabled multigrid solvers within several application codes.

## [03924] Implications of multiphysics problems in multigrid methods from a linear algebra view point

**Format :** Talk at Waseda University

**Author(s) :** Matthias Bolten (University of Wuppertal)

**Abstract :** Multiphysics problems require special attention in multigrid methods, as standard methods often do not converge. To overcome this, different approaches have been considered, e.g. special smoothers and special grid transfer and coarse grid selection. We are studying methods for block matrices, as they arise when systems of PDEs are considered. Different approaches for block matrices are presented, including block smoothers as well as analysis of multigrid methods resulting in requirements on grid transfer operators.

## [03818] Parallel scalable solvers for Helmholtz problems

**Format :** Talk at Waseda University

**Author(s) :** Cornelis Vuik (Delft University of Technology) Jinqiang Chen (Delft University of Technology) Vandana Dwarka (Delft University of Technology)

**Abstract :** A matrix-free, parallel multi-level deflation preconditioning method is proposed for Helmholtz problems. The method integrates the geometric multi-grid-based Complex Shifted Laplace Preconditioner (CSLP) and higher-order deflation, employing re-discretization schemes derived from Galerkin coarsening approach for a matrix-free parallel implementation. The method shows close to wavenumber-independent convergence and satisfactory strong, and weak parallel scalability. Numerical experiments demonstrate the effectiveness of our approach for complex mo problems, solving large-scale heterogeneous Helmholtz problems with minimized pollution error.

## [02018] Reynolds-robust preconditioners for the stationary incompressible viscoresistive MHD equations

**Format :** Talk at Waseda University

**Author(s) :** Patrick Emmet Farrell (University of Oxford) Fabian Laakmann (University of Oxford)

**Abstract :** We present an augmented Lagrangian preconditioner for the incompressible viscoresistive equations of magnetohydrodynamics. For stationary problems, our solver achieves robust performance with respect to the Reynolds and coupling numbers. We extend our method to fully implicit methods for time-dependent problems. Our approach relies on specialized parameter-robust multigrid methods for the hydrodynamic and electromagnetic blocks. The scheme ensures exactly divergence-free approximations of both the velocity and the magnetic field up to solver tolerances.

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01054 (2/3) : 4E @E507 [Chair: Alexander Heinlein]

## [04232] Robust nonlinear domain decomposition methods for problems with micro-heterogeneous structures

**Format :** Talk at Waseda University

**Author(s) :** Alexander Heinlein (Delft University of Technology (TU Delft))Axel Klawonn (University of Cologne)Martin Lanser (University of Cologne)

**Abstract :** Nonlinear domain decomposition methods (DDMs) are efficient alternatives to classical Newton-Krylov-DDMs.

In contrast to the latter ones, in nonlinear DDMs, the nonlinear partial differential equation is decomposed into subdomains before linearization, which often improves the nonlinear convergence behavior. To obtain robustness applying nonlinear DDMs to heterogeneous multiscale or multiphysics problems, a global and coarse second level should be included. In this talk, several two-level nonlinear Schwarz methods for heterogeneous problems are discussed and compared.

## [05039] Immersed Mesh Methods for Coupled Multiphysics Problems

**Format :** Talk at Waseda University

**Author(s) :** Rolf Krause (Euler Institute, USI, Lugano)Patrick Zulian (Euler Institute, USI, Lugano)Maria Nestola (Euler Institute, USI, Lugano)

**Abstract :** We present overlapping domain decomposition methods coupling different discretizations in the volume, along surfaces, or between surfaces and volumes. Central element of our approach is a massively parallel discrete  $L^2$  projection, which allows for stable variational transfer between different physical models. Examples from fluid structure interaction (FSI), i.e. artificial heart valves, or flow in fracture networks, as well as from contact mechanics coupled with FSI illustrate our approach.

## [04600] Towards a scalable multilevel domain decomposition solver for immersed boundary finite element method

**Format :** Talk at Waseda University

**Author(s) :** Jakub Sistek (Institute of Mathematics of the Czech Academy of Sciences)

**Abstract :** We develop multilevel balancing domain decomposition by constraints (BDDC) method tailored to the solution of the linear systems arising in the context of immersed boundary FEM with parallel adaptive grid refinement. A crucial challenge is presented by fragmenting of subdomains. We present these concepts, the challenges, our implementation, and numerical results for the Poisson problem on complex geometries from engineering. This is joint work with Fehmi Cirak, Eky Febrianto, Matija Kecman, and Pavel Kus.

## [03836] Co-Design of Modelling and Monolithic Overlapping Schwarz Solvers in Chemo-Mechanics

**Format :** Talk at Waseda University

**Author(s) :** Friederike Röver (TU Bergakademie Freiberg)Bjoern Kiefer (TU Bergakademie Freiberg)Stefan Prüger (TU Bergakademie Freiberg)Oliver Rheinbach (TU Bergakademie Freiberg)

**Abstract :** The focus of this talk is the co-design of the variational formulations arising from model problems in chemo-mechanics and parallel iterative solvers from domain decomposition.

We choose the FROSCh framework of the Trilinos Software library as a parallel solver. It contains a parallel implementation of the GDSW preconditioner, which allows an algebraic construction.

We present results applying FROSCh to a fully coupled deformation-diffusion boundary value problem of a swelling hydrogel. For the FE-implementation, we use the deal.II software library and incorporate FROSCh as a solver framework.

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01054 (3/3) : 5B @E507 [Chair: Alexander Heinlein]

## [03397] A tensor-preserving domain decomposition preconditioner for high-order implicit methods

**Format :** Talk at Waseda University

**Author(s) :** Jing-Yuan Wang (University of Macau)Yingzhi Liu (University of Macau)Xiao-Chuan Cai (University of Macau)

**Abstract :** We investigate high-order block implicit methods for solving parabolic and unsteady Stokes problems, including the fully implicit Runge-Kutta method as a special case. These methods provide high accuracy with relatively large time step size, but the large, often nonsymmetric, and highly ill-conditioned stiffness matrix limits its practical use. To overcome this, we propose one- and two-level tensor-preserving domain decomposition preconditioners. Numerical experiments show the effectiveness and scalability of this approach for parabolic and Stokes flows.

## [01058] Recent advances in stochastic nonlinear dynamics: modeling, data analysis

**Session Time & Room :**

01058 (1/3) : 2D (Aug.22, 15:30-17:10) @E502

01058 (2/3) : 2E (Aug.22, 17:40-19:20) @E502

01058 (3/3) : 3C (Aug.23, 13:20-15:00) @E502

**Type :** Proposal of Minisymposium

**Abstract :** Stochasticity, nonlinearity and complexity can be found and used in many different fields, including the natural sciences such as mechanics, physics, biology, neuroscience as well as technology and engineering fields such as aeronautics, astronautics, information theory and computer science. The symposium focuses on the stochastic modeling and data analysis in nonlinear dynamical system. The contributions cover various fields such as Brownian motion, Levy process, and fractional Brownian motion et al and applications, data analysis methods and techniques combining complex systems science and machine learning. This symposium provides a forum to discuss science, strengthen relationships, create new contacts and gain a direct experience of new progresses in stochastic modeling and data analysis.

**Organizer(s) :** Yong Xu, Bin Pei, Yongge Li

**Classification :** 60H10, Stochastic ordinary differential equations

**Minisymposium Program :**

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01058 (1/3) : 2D @E502 [Chair: Xiaole Yue]

## [02085] Almost sure averaging for fast-slow stochastic differential equations via controlled rough path

**Format :** Talk at Waseda University

**Author(s) :** Bin PEI (Northwestern Polytechnical University)Yong Xu (Northwestern polytechnical university)

**Abstract :** We apply the averaging method to a coupled system consisting of two differential equations which has a slow component driven by fractional Brownian motion (FBM) with the Hurst parameter  $\frac{1}{3} < H_1 \leq \frac{1}{2}$  and a fast component driven by additive FBM with the Hurst parameter  $\frac{1}{3} < H_2 \leq \frac{1}{2}$ . The main purpose is to show that the slow component of such a couple system can be described by a stochastic differential equation with averaged coefficients. Our main result deals with an averaging procedure which proves that the slow component converges almost surely to the solution of the corresponding averaged equation using the approach of time discretization and controlled rough path. To do this we generate a stationary solution by a exponentially attracting random fixed point of the random dynamical system generated by the fast component.

## [01488] Discrete-time Approximation of Partially Observed Stochastic Optimal Control Problem

**Format :** Talk at Waseda University

**Author(s) :** Yunzhang Li (Fudan University)

**Abstract :** In this talk, we study a class of stochastic optimal control problems under partial observation by discrete-time control problems. To establish a convergence result, we adapt the weak convergence technique together with the notion of relaxed control rule. With a well chosen discrete-time control system, we provide an implementable numerical algorithm to approximate the value. We illustrate our convergence result by numerical experiments on a partially observed control problem in a linear quadratic setting.

## [03981] Large deviations for a slow-fast McKean-Vlasov model with jumps

**Format :** Talk at Waseda University

**Author(s) :** Xiaoyu YANG (Northwestern Polytechnical University)Yong Xu (Northwestern polytechnical university)

**Abstract :** We aim to investigate large deviations for a slow-fast McKean-Vlasov system with jumps. Based on the variational framework of the McKean-Vlasov system with jumps, it is turned into weak convergence for the controlled system. Different from the general case, the controlled system is related to the distribution of the original system, which causes difficulties. To solve it, the combination of asymptotic of original system and averaging principle is employed efficiently.

## [02182] Recent advances in stochastic nonlinear dynamics: modeling, data analysis

**Format :** Online Talk on Zoom

**Author(s) :** Zi-Fei Lin (Xi 'an University of Finance and Economics)Yan-Ming liang (Xi 'an University of Finance and Economics)Jia-Li Zhao (Xi 'an University of Finance and Economics)Jiao-Rui Li (Xi 'an University of Finance and Economics)Kapitaniak Tomasz (Lodz University of Technology)

**Abstract :** Predicting strongly noise-driven dynamic systems has always been a difficult problem due to their chaotic properties. In this study, we investigated the prediction of dynamic systems driven by strong noise intensities, which proves that deep learning can be applied in diverse fields. This is the first study that uses deep learning algorithms to predict dynamic systems driven by strong noise intensities. We examined the effect of hyperparameters in deep learning and introduced an improved algorithm for prediction. Several numerical examples are presented to illustrate the performance of the proposed algorithm, including the Lorenz system and the Rossler system driven by noise intensities of 0.1, 0.5, 1, and 1.25. All the results suggest that the proposed improved algorithm is feasible and effective for predicting strongly noise-driven dynamic systems. Furthermore, the influences of the number of Neurons, the Spectral Radius, and the Regularization Parameters are discussed in detail. These results indicate that the performances of the machine learning techniques can be improved by appropriately constructing the neural networks.

01058 (2/3) : 2E @E502 [Chair: Bin Pei]

## [02193] Response prediction of dynamical systems with the GCM-DL method

**Format :** Talk at Waseda University

**Author(s) :** Xiaole Yue (Northwestern Polytechnical University)Yong Xu (Northwestern polytechnical university)Xiaocong Liu (Northwestern Polytechnical University)Yue Zhao (Northwestern Polytechnical University)

**Abstract :** Generalized cell mapping method based on deep learning is proposed which can predict responses of dynamical systems from experimental data with part of information about physical model. This method trains the neural network model from a small amount of experimental data and obtains the potential dynamic model. The global characteristics of system are analyzed by GCM method. By introducing deconvolution layer and image super-resolution, the probability density function of stochastic dynamic system response is estimated.

## [02190] Complex dynamics of a conceptual airfoil structure with consideration of extreme flight conditions

**Format** : Talk at Waseda University

**Author(s)** : Qi Liu (Tokyo Institute of Technology)

**Abstract :** An aircraft in practice serves under extreme flight conditions, that will have a substantial impact on its flight safety. Understanding dynamics of airfoil structure of an aircraft subjected to severe load conditions is thus extremely valuable and necessary. In this study, we will explore the complicated dynamical behaviors of a conceptual airfoil excited by an external harmonic force and an extreme random load. Importantly, such an extreme random load is portrayed by a non-Gaussian Lévy noise with a heavy-tailed feature. We theoretically deduce amplitude-frequency equations associated with the deterministic airfoil system. We observe excellent agreements between the analytical solutions and the numerical ones, as well as bistable behaviors. Besides, the effects of the extreme random load on the airfoil system are thoroughly investigated. Interestingly, within the bistable regime, the extreme random load can lead to stochastic transition and stochastic resonance. Due to its heavy-tailed nature, the Lévy noise would increase the possibility of a highly unexpected stochastic transition behavior between desirable low-amplitude and catastrophic high-amplitude oscillations compared with the Gaussian scenario. Such vibration patterns might damage or destroy the airfoil structure, which will put an aircraft in great danger. All the findings would be helpful in ensuring the flight safety and enhancing the strength and reliability of airfoil structure operating at extreme flight conditions.

[02205] Pattern Dynamics of Higher Order Reaction-Diffusion network

**Format** : Talk at Waseda University

**Author(s)** : Jianwei Shen (North China University of Water Resources and Electric Power)

**Abstract :** In this paper, we will investigate the pattern dynamics of higher order reaction-diffusion network by group interactions and prove the interplay between different orders of interaction can affect the emergence of turing patterns. Our results try to the mechanism of many body interaction on complex network.

## [02243] Three occurrence mechanisms of extreme events in stochastic dynamical systems

**Format :** Online Talk on Zoom

**Author(s)** : Yongge Li (Northwestern Polytechnical University)Dan Zhao (Northwestern Polytechnical University)Yong Xu (Northwestern polytechnical university)

**Abstract :** In this work, three mechanisms for the occurrence of extreme events in stochastic dynamical systems are given. Firstly, for systems with a bifurcation structure, if the difference of the branches at the bifurcation point is large, then a time-varying amplitude of the external periodic excitation is able to induce an extreme event. This is verified in the rolling motion of a ship system. Secondly, for systems with rare attractors, a random pulse excitation, such as Poisson white noise, is able to drive the system to escape from the basin of general attractor to that of rare attractor. However, the basin of rare attractor is so small that the system will go back to the general state immediately. Such a kind of transition is also extreme event. Finally, an extreme excitation can also generate extreme event, such as the Lévy noise. In such cases, it does not require much about the systems, but the extreme excitations work. These results provide theoretical guidance for further prediction and avoidance of extreme events.

01058 (3/3) : 3C @E502 [Chair: Qi Liu]

## [02092] Homogenization of the two dimensional singular polymer measure

**Format :** Online Talk on Zoom

**Author(s)** : Huanyu Yang (Free University of Berlin)

**Abstract :** We consider the SDE on \$

[0,n]\$:

```
\begin{equation}
\left\langle \begin{aligned}
&\partial_t^{\alpha} u(t) - \Delta u(t) + f(u(t)) = 0, \\
&u(0) = u_0
\end{aligned} \right.

```

```
Z_0^n&=x,
```

```
\end{aligned}
```

```
\right.
```

```
\end{equation}
```

where  $B$  is the standard Brownian motion and  $h$  is the solution to KPZ equation driven by space-white noise  $\xi$  on  $\mathbb{T}^2$ .

The law of  $Z^n$  is the same as the law of the coordinate process under the singular polymer measure  $Q^n$  constructed by Cannizzaro and Chouk:

```
\begin{equation}
```

```
Q^n(d\omega)=\frac{1}{U(n)}\exp\left(\int_0^n\left(\langle \omega(s), h(s) \rangle - \frac{1}{2}\|h(s)\|^2\right)ds + \sqrt{n}\int_0^n dW(s)\right)
```

```
\right)\mathbb{W}(d\omega),
```

```
\end{equation}
```

where  $\mathbb{W}$  is the Wiener measure on  $\mathcal{C}$

**[0,\infty),\mathbb{R}). By decomposing the drift term  $h$**

*into a singular time-homogeneous and a smooth time-dependent term, we prove that*

$\left(\frac{1}{\sqrt{n}}Z^{nt}\right)_{t \geq 0}$

**[0,1] converges to a Brownian motion.**

This is the joint work with Nicolas Perkowski.

## [01060] Exploring Arithmetic and Data Representation Beyond the Standard in HPC

**Session Time & Room :**

01060 (1/3) : 1C (Aug.21, 13:20-15:00) @E803

01060 (2/3) : 1D (Aug.21, 15:30-17:10) @E803

01060 (3/3) : 1E (Aug.21, 17:40-19:20) @E803

**Type :** Proposal of Minisymposium

**Abstract :** This mini-symposium explores the potential of utilizing arithmetic operations and data representations other than FP32 (single-precision) and FP64 (double-precision) in numerical computations with HPC. Such attempts include not only higher or lower floating-point precision, but also integer representation, error handling, rounding, etc., and are intended not only for performance but also for quality and reliability of computations. We explore various angles of this challenge, from low-level implementations to applications.

**Organizer(s) :** Daichi Mukunoki, Naohito Nakasato, Tomonori Kouya

**Classification :** 68M99, 65Y04, 65Y05

**Minisymposium Program :**

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01060 (1/3) : 1C @E803 [Chair: Daichi Mukunoki]

## [01783] FP-ANR: A representation format to handle floating-point cancellation at run-time

**Author(s) :** David DEFOUR (Universite de Perpignan)

**Abstract :** When dealing with floating-point numbers there are several sources of error which can drastically reduce the numerical quality of computed results. Among those errors, the loss of significance, or cancellation, occurs during for example the subtraction of two nearly equal numbers. In this article, we propose a representation format named Floating-Point Adaptive Noise Reduction (FP-ANR). This format embeds cancellation information directly into the floating-point representation format thanks to a dedicated pattern. With this format, unsignificant trailing bit lost during cancellation are removed from every manipulated floating-point number. The immediate consequence is that it increases the numerical confidence of computed values. The proposed representation format

part\_2

corresponds to a simple and efficient implementation of significance arithmetic based and compatible with the IEEE-754 standard.

## [01812] Precision autotuning using stochastic arithmetic

**Author(s)** : Quentin Ferro (Sorbonne University)Stef Graillat (Sorbonne University)Thibault Hilaire (Sorbonne University)Fabienne Jezequel (Sorbonne University)

**Abstract** : We present PROMISE, a tool that makes it possible to provide a mixed precision version of a program by taking into account the requested accuracy on the computed results. With PROMISE the numerical quality of results is verified using Discrete Stochastic Arithmetic that enables one to estimate round-off errors. PROMISE has been used for floating point auto-tuning on neural networks to lower their precision while keeping an accurate output.

## [01839] Implementation of highly optimized multiple precision BLAS: Strassen vs. Ozaki scheme

**Author(s)** : Tomonori Kouya (Shizuoka Institute of Science and Technology)

**Abstract** : We have already developed a highly optimized extended multiple precision basic linear algebra subprogram library using various technologies such as AVX2 and OpenMP. In particular, Strassen algorithm and Ozaki scheme we employed are distinctive methods for accelerating matrix multiplication. In this talk, we describe the software structure of our library and highlight the advantages and disadvantages of Strassen algorithm and Ozaki scheme through benchmark tests using fixed- and arbitrary-precision floating-point arithmetic.

## [03869] Accelerating 128-bit Matrix Multiplication for Applications using FPGAs

**Author(s)** : Fumiya Kono (Shizuoka Institute of Science and Technology)

**Abstract** : General Matrix Multiplication (GEMM) is a core of various scientific applications. Since the requirement for the number of bits representing floating-point numbers depends on individual applications, the precision of GEMM is critical. Particularly, Semidefinite Programming requires higher precision, such as binary128. We researched methods of accelerating GEMM in binary128 using FPGAs because arithmetic in binary128 was very slow without hardware unit support. This talk presents an evaluation of our designs on several Intel FPGAs.

01060 (2/3) : 1D @E803 [Chair: Naohito Nakasato]

## [04191] Multiple Integer Divisions with an Invariant Dividend

**Author(s)** : Daisuke Takahashi (University of Tsukuba)

**Abstract** : In this talk, we propose an algorithm for multiple integer divisions with an invariant dividend and monotonically increasing or decreasing divisors.

In such multiple integer divisions, we show that if the dividend and divisors satisfy a certain condition, then if only one quotient is calculated by division first, the remaining quotients can be obtained by correcting the previously calculated quotients at most once.

## [04628] Reduced-Precision Data Representation on Sparse Matrix-Vector Multiplications

**Author(s)** : Daichi Mukunoki (RIKEN Center for Computational Science)Masatoshi Kawai (Nagoya University)Toshiyuki Imamura (RIKEN Center for Computational Science)

**Abstract** : In sparse iterative solvers, data and arithmetic precision affect convergence and solution accuracy, and their precision can be optimized. There is a demand for its kernel, sparse matrix vector multiplication (SpMV), with different precision. Due to its memory-intensive nature, SpMV could benefit from low-precision floating-point formats to improve performance. In this talk, we demonstrate the performance of our SpMV implementations on CPU and GPU, allowing precision adjustment in 8-bit increments from 16 to 64 bits.

## [04862] High-performance multidimensional integration

**Author(s)** : Elise Helene de Doncker (Western Michigan University)

**Abstract** : Techniques for parallel multidimensional integration will be presented, with applications to Feynman loop integrals

in high energy physics. Integrand singularities are addressed with adaptive region partitioning, transformations, and convergence acceleration via linear or nonlinear extrapolation.

Parallel implementations are commonly layered over a platform that interfaces with the underlying computer architecture, including MPI (Message Passing Interface), OpenMP for iterated multi-threaded integration, and CUDA kernels supporting integrand evaluation for lattice type rules on thousands of GPU CUDA cores.

## [04875] Introducing MPLAPACK 2.0.1: An Extension of BLAS and LAPACK for Multiple Precision Computation

**Author(s)** : Maho Nakata (RIKEN)

**Abstract** : MPLAPACK, a multiple-precision extension of LAPACK, offers enhanced numerical linear algebra capabilities. Translated from Fortran 90 to C++ using FABLE, MPLAPACK 2.0.1 supports MPBLAS, real and complex versions, and all LAPACK features except mixed-precision routines. Porting legacy C/C++ numerical codes is straightforward, and it supports various numerical libraries for diverse precision levels. MPLAPACK offers OpenMP acceleration for some routines and CUDA support for specific double-double versions. Achieving impressive performance, MPLAPACK is available under the 2-clause BSD license on GitHub.

01060 (3/3) : 1E @E803 [Chair: Tomonori Kouya]

## [04912] Evaluation of various arithmetic for linear algebra on GPU and FPGA

**Author(s)** : Naohito Nakasato (University of Aizu)

**Abstract** : We present the evaluation of various non-standard floating-point (FP) arithmetic for linear algebra. We accelerate matrix multiplication in 128-bit FP arithmetic on both GPU and FPGA. Also we evaluate other FP format such as POSIT and reduced precision FP arithmetic. We discuss the energy efficiency and the numerical accuracy of the non-standard FP arithmetic on GPUs and FPGA accelerators for dense matrices.

## [05094] Using quad-precision numbers for preconditioner of domain decomposition method

**Author(s)** : Hiroshi Kawai (Toyo University)Masao Ogino (Daido University)Ryuji Shioya (Toyo University)

**Abstract** : Domain decomposition method with BDD preconditioner is one of the effective parallelization methods for the finite element method. Coarse grid correction in BDD handles a medium-sized linear system, which could be bottleneck in parallel environment. To accelerate this step, the inverse approach is adopted. It replaces forward and back substitution to parallel matrix vector multiplication. Double-double is utilized to preserve the accuracy of the inverse matrix.

## [01063] Challenges in biomathematical modeling and control

**Session Time & Room :**

01063 (1/3) : 1C (Aug.21, 13:20-15:00) @A206

01063 (2/3) : 1D (Aug.21, 15:30-17:10) @A206

01063 (3/3) : 1E (Aug.21, 17:40-19:20) @A206

**Type** : Proposal of Minisymposium

**Abstract** : In biomathematics, theoretical and data modeling showed to be big challenges, both at the macroscopic and microscopic levels. Complex networks are proved to be a rather powerful theoretical tools in epidemics, neuroscience, protein functions, ecology and cancer. When considering space-time analysis of big data, we have at

part\_2

our disposal a variety of methods, wavelets, Bayesian, Topological Data Analysis, Cross-entropy, Fuzzy logic, among others. The choice of a method is linked to the kind of questions we want to target.

The emergency experienced with pandemics showed also the importance of being able to make predictions and to develop methods of control.

**Organizer(s)** : Stefanella Boatto, Bernard Cazelles, Ludovick Gagnon

**Classification** : 92D40, 55N31, 05C82, 92D20, 92D30, complex networks, topological data analysis, networks in neurosciences, mathematical ecology, epidemiological modelling, cancer modelling, genomics

**Minisymposium Program :**

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01063 (1/3) : 1C @A206

## [05271] Analyzing infectious disease dynamics: the challenge of non-stationarity

**Author(s)** : Bernard Cazelles (IBENS CNRS INSERM)

**Abstract** : The spread of disease through human populations is complex. The characteristics of disease propagation evolve with time, as a result of a multitude of environmental and anthropic factors, including social distancing. This non-stationarity is a key factor in the complexity of disease propagation.

In the absence of appropriate external data sources, to correctly describe disease propagation, I propose a flexible methodology, based on stochastic models for disease dynamics, and on Brownian processes for parameter evolution. Using such a diffusion process has the advantage of not requiring a specific mathematical function for the parameter dynamics. Coupled with Bayesian inference using particle MCMC, this approach allows us to reconstruct both the time evolution of some key parameters of an epidemiological dynamic and its incidence.

I will demonstrate the efficiency of this methodology on toy epidemiological models where the parameters and the observation process are known, and also on more complex epidemics, such as flu, dengue and COVID-19.

## [05319] Models of mosquito population control strategies for fighting against arboviruse

**Author(s)** : Michel Duprez (Inria)Luis Almeida (Inria)Yves Dumont (CIRAD - University of Pretoria)yannick Privat (Université de Strasbourg)Nicolas Vauchelet (Université Paris 13)

**Abstract** : In the fight against vector-borne arboviruses, an important strategy of control of epidemic consists in controlling the population of the vector, Aedes mosquitoes in this case. Among possible actions, a technique consist in releasing sterile mosquitoes to reduce the size of the population (Sterile Insect Technique). This talk is devoted to studying the issue of optimizing the dissemination protocol for each of these strategies, in order to get as close as possible to these objectives. Starting from a mathematical model describing the dynamic of a mosquitoes population, we will study the control problem and introduce the cost function standing for sterile insect technique. In a second step, we will consider a model with several patches modeling the spatial repartition of the population. Then, we will establish some properties of these two optimal control problems. Finally, we will illustrate our results with numerical simulations.

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01063 (2/3) : 1D @A206

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01063 (3/3) : 1E @A206

## [01064] Recent Advances on Manifold Optimization

**Session Time & Room :**

01064 (1/3) : 3D (Aug.23, 15:30-17:10) @E605

01064 (2/3) : 3E (Aug.23, 17:40-19:20) @E605

01064 (3/3) : 4C (Aug.24, 13:20-15:00) @E605

**Type :** Proposal of Minisymposium

**Abstract :** Manifold optimization has been developing remarkably with its rich theory and a wide variety of applications. This minisymposium aims to pioneer state-of-the-art in the field. The talks include optimization algorithms on manifolds, e.g., Riemannian adaptive and interior point methods, ADMM, local stochastic algorithms, a CG method for multiobjective optimization, and an augmented Lagrangian method based on sequential optimality conditions. Furthermore, efficient optimization on specific manifolds such as Grassmann and Stiefel manifolds and the manifold of fixed-rank positive-semidefinite matrices, and applications to practical problems, e.g., problems under differential privacy, low-rank matrix optimization problems, and design of tight minimum-sidelobe windows, are addressed.

**Organizer(s) :** Hiroyuki Sato, Kensuke Aihara

**Classification :** 65K05, 90C06, 90C30, 90C48, 90C90

**Minisymposium Program :**

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01064 (1/3) : 3D @E605 [Chair: Kensuke Aihara]

## [04372] Sequential optimality conditions for nonlinear optimization on Riemannian manifolds and a globally convergent augmented Lagrangian method

**Format :** Talk at Waseda University

**Author(s) :** Yuya Yamakawa (Kyoto University)Hiroyuki Sato (Kyoto University)

**Abstract :** Recently, the approximate Karush–Kuhn–Tucker (AKKT) conditions, also called the sequential optimality conditions, have been proposed for nonlinear optimization in Euclidean spaces, and several methods to find points satisfying such conditions have been developed by researchers. These conditions are known as genuine necessary optimality conditions because all local optima satisfy them with no constraint qualification (CQ). In this paper, we extend the AKKT conditions to nonlinear optimization on Riemannian manifolds and propose an augmented Lagrangian (AL) method that globally converges to points satisfying such conditions. In addition, we prove that the AKKT and KKT conditions are indeed equivalent under a certain CQ. Finally, we examine the effectiveness of the proposed AL method via several numerical experiments.

## [04682] Nonlinear conjugate gradient method for vector optimization on Riemannian manifolds

**Format :** Talk at Waseda University

**Author(s) :** Kangming Chen (Kyoto University)Hiroyuki Sato (Kyoto University)Ellen Hidemi Fukuda (Kyoto University)

**Abstract :** In this research, we propose a conjugate gradient descent algorithm for vector optimization on Riemannian manifolds. We extend the concepts of Wolfe conditions and Zoutendjik conditions to Riemannian manifolds. The convergence of the proposed method is proved for different choices of the parameter beta, including the Riemannian extension of Fletcher-Reeves, Conjugate Descent, and Dai-Yuan. Numerical experiments are conducted to validate the proposed method.

## [04852] Gauss-Southwell type descent methods for low-rank matrix optimization

**Format :** Talk at Waseda University

**Author(s) :** Guillaume Olikier (Université Catholique de Louvain)André Uschmajew (University of Augsburg)Bart Vandereycken (University of Geneva)

**Abstract :** We consider gradient-related methods for low-rank matrix optimization with a smooth strongly convex cost function. The methods operate on single factors and share aspects of both alternating and Riemannian optimization. We compare two possible choices for the search directions based on Gauss-Southwell type selection rules: one using the gradient of a factorized non-convex formulation, the other using the Riemannian gradient. Both methods provide convergence guarantees for the gradient that are analogous to the unconstrained case.

## [03269] Min-max optimization on manifolds

**Format :** Online Talk on Zoom

**Author(s) :** Bamdev Mishra (Microsoft )

**Abstract :** In this talk, we discuss some recent algorithms on min-max optimization problems over Riemannian manifolds.

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01064 (2/3) : 3E @E605 [Chair: Hiroyuki Sato]

## [03743] Design of Tight Minimum-Sidelobe Windows via Optimization on Oblique Manifolds

**Format :** Online Talk on Zoom

**Author(s) :** Daichi Kitahara (Osaka University)Kohei Yatabe (Tokyo University of Agriculture and Technology)

**Abstract :** The short-time Fourier transform (STFT), or the discrete Gabor transform (DGT), has been widely utilized in signal analysis and processing. For noise-robust STFT/DGT domain signal processing, windows used in STFT/DGT are desired to be tight. In this talk, we propose to design tight windows minimizing the sidelobe energy. It is expressed as the maximization of Rayleigh quotients on oblique manifolds. We apply the Riemannian Newton's method to obtain the optimal tight windows by several iterations.

## [04008] The Bures-Wasserstein geometry of the manifold of fixed-rank positive-semidefinite matrices

**Format :** Online Talk on Zoom

**Author(s) :** Estelle Massart (UCLouvain)Pierre-Antoine Absil (UCLouvain)

**Abstract :** We explore the well-known identification of the manifold of rank  $p$  positive-semidefinite matrices of size  $n$  with the quotient of the set of full-rank  $n$ -by- $p$  matrices by the orthogonal group in dimension  $p$ . The induced metric corresponds to the Wasserstein metric between centered degenerate Gaussian distributions, and is a generalization of the Bures–Wasserstein metric on the manifold of positive-definite matrices.

## [02861] Cayley parametrization strategy for optimization over the Stiefel manifold

**Format :** Talk at Waseda University

**Author(s) :** Keita Kume (Tokyo Institute of Technology)Isao Yamada (Tokyo Institute of Technology)

**Abstract :** We introduce the basic idea behind the adaptive localized Cayley parametrization strategy for optimization over the Stiefel manifold. The proposed adaptive strategy can mitigate slow convergence caused by singular-points of the naive Cayley parametrization. Unlike the so-called retraction-based strategy, the proposed strategy can utilize directly many powerful Euclidean optimization algorithms. For a certain class of optimization algorithms combined with the proposed parametrization strategy, we also explain briefly an idea for their unified convergence analyses.

## [02851] Accelerated gradient methods on the Grassmann and Stiefel manifolds

**Format :** Talk at Waseda University

**Author(s) :** Xiaojing Zhu (Shanghai University of Electric Power)

**Abstract :** In this talk we extend a nonconvex version of Nesterov's accelerated gradient method to optimization over the Grassmann and Stiefel manifolds. We propose an exponential-based AG algorithm for the Grassmann manifold and a retraction-based AG algorithm that exploits the Cayley transform for both of the Grassmann and Stiefel manifolds. Global rates of convergence of our algorithms are analyzed under reasonable assumptions. Details of computing some geometric objects as ingredients of our algorithms are also discussed.

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01064 (3/3) : 4C @E605 [Chair: Xiaojing Zhu]

## [04571] A Riemannian ADMM

**Format :** Online Talk on Zoom

**Author(s) :** Shiqian Ma (Rice University)

**Abstract :** We consider a class of Riemannian optimization problems where the objective is the sum of a smooth function and a nonsmooth function, considered in the ambient space. This class of problems finds important applications in machine learning and statistics such as the K-means clustering, sparse spectral clustering, and orthogonal dictionary learning. We propose a Riemannian alternating direction method of multipliers to solve this class of problems. Our algorithm adopts easily solvable subproblems in each iteration. The iteration complexity of the proposed algorithm for obtaining an  $\epsilon$ -stationary point is analyzed under mild assumptions. Numerical experiments are conducted to demonstrate the advantage of the proposed method.

## [04455] Local stochastic algorithms for Riemannian optimization

**Format :** Online Talk on Zoom

**Author(s) :** Sam Davanloo Tajbakhsh (The Ohio State University)

**Abstract :** We consider optimizing a function available through its first-order stochastic oracle over a Riemannian manifold in a distributed setting with the coordination of a central server. We develop local stochastic approximation methods that perform multiple local stochastic updates in parallel on different clients and merge them in some intervals. Theoretical convergence results in different optimization and communication settings will be presented.

## [03649] Riemannian Interior Point Methods for Constrained Optimization on Manifolds

**Format :** Talk at Waseda University

**Author(s) :** Zhijian Lai (University of Tsukuba)Akiko Yoshise (University of Tsukuba)

**Abstract :** We extend the classical primal-dual interior point method from the Euclidean setting to the Riemannian one. Our method, named the Riemannian interior point method (RIPM), is for solving Riemannian constrained optimization problems. We establish its locally superlinear and quadratic convergence under the standard assumptions. Moreover, we show its global convergence when it is combined with a classical line search. Numerical experiments show the stability and efficiency of our method.

## [03887] Riemannian Adaptive Optimization Algorithms and Their Applications

**Format :** Talk at Waseda University

**Author(s) :** Hiroyuki Sakai (Meiji University)Hideaki Iiduka (Meiji University)

**Abstract :** We will talk about Riemannian adaptive optimization algorithms to solve the Riemannian stochastic optimization problems. In Euclidean space, adaptive optimization algorithms, such as AdaGrad, Adam, Adadelta, and AMSGrad, are widely used. However, adaptive optimization algorithms cannot be naturally extended to general Riemannian manifolds, due to the absence of a canonical coordinate system.

We introduce the ways to generalize adaptive optimization algorithms to Riemannian manifolds and consider their applications.

# [01065] Mathematics and its Applications of Risk and Decision

**Session Time & Room :** 4E (Aug.24, 17:40-19:20) @D501

**Type :** Proposal of Minisymposium

**Abstract :** In the age of uncertainty highlighted by events such as the financial crisis and the outbreak of COVID-19, policy makers need to acquire a holistic yet rigorous understanding of decision making under risk. This symposium aims to bring together academic researchers of diverse background to showcase the latest development of the mathematical theories and applications for risk and decision. The covered topics include stochastic control, optimal decision-making, model uncertainty and their applications in fields like economics and insurance. The collective effort of the expert speakers from this symposium will constitute impactful decision protocols and policy implications.

**Organizer(s) :** Alex S.L. Tse, Andrea Macrina

**Classification :** 91B06, 93E20, 91B05, 91G15, 91G05

**Minisymposium Program :**

01065 (1/1) : 4E @D501 [Chair: Alex S.L. Tse]

## [04299] Optimal reinsurance with multivariate risks and dependence uncertainty

**Format :** Talk at Waseda University

**Author(s) :** Tolulope Rhoda Fadina (University of Essex)Tolulope Fadina (University of Essex)

**Abstract :** We study the optimal reinsurance design from the perspective of an insurer with multiple lines of business, where the

reinsurance is purchased by the insurer for each line of business respectively. For the risk vector generated by the multiple lines of business, we suppose that the marginal distributions are fixed, but the dependence structure between

these risks is unknown. Due to the unknown dependence structure, the optimal strategy is investigated for the worst-case scenario. We consider two types of risk measures: Value-at-Risk (VaR) and Range-Value-at-Risk including Expected Shortfall as a special case, and general premium principles satisfying certain conditions. To be more

practical, the minimization of the total risk is conducted with both budget constraints and expected profit constraints.

For the VaR-based model with only two risks, it turns out that the limited stop-loss reinsurance treaty is optimal for each line of business. For the model with more than two risks, we obtain two types of optimal reinsurance strategies if the marginals have convex or concave distributions on their tail parts by constraining the ceded loss functions to be convex or concave.

## [04329] Irreversible consumption habit under ambiguity: Singular control and optimal G-stopping time

**Format :** Talk at Waseda University

**Author(s) :** HOI YING WONG (The Chinese University of Hong Kong)Kyunghyun Park (Nanyang Technological University)Kexin Chen (The Hong Kong Polytechnic University)

**Abstract :** Consider robust utility maximization with an irreversible consumption habit, where an agent concerned about model ambiguity is unwilling to decrease consumption and must simultaneously contend with a disutility (i.e., an adjustment cost) due to a consumption increase. While the optimization is a robust analog of singular control problems over a class of consumption-investment strategies and a set of probability measures, it is a new formulation that involves non-dominated probability measures of the diffusion process for the underlying assets in addition to singular controls with an adjustment cost. This paper provides a novel connection between the singular controls in the optimization and the optimal G-stopping times in a G-expectation space, using a duality theory. This connection enables to derive the robust consumption strategy as a running maximum of the stochastic boundary, which is characterized by a free boundary arising from the optimal G-stopping times. The duality, which relies on arguments based on reflected G-BSDEs, is achieved by verifying the first-order optimality conditions for the singular control, the budget constraint equation for the robust strategies, and the worst-case realization under the non-dominated measures.

## [05330] On/Off Shore Currency Rate Discrepancy

**Format :** Talk at Waseda University

**Author(s) :** Samuel Drapeau (Shanghai jiao Tong university )Xuan Tao (Shanghai Jiao Tong University)

**Abstract :** Most developing countries (especially in Asia) adopted a tight control of foreign capital in order to protect their economy from abrupt capital outflows in period of crisis.

As those economies developed and opened up to foreign financial investment, they often set up off shore currency exchange markets to facilitate the transfer of capital.

This is for instance the case of China where the on shore rmb (CNY) was complemented with an off shore market for trading this currency (CNH).

Theoretically, the face value from a domestic viewpoint of the currency is the same regardless of on/off shore origin.

And indeed, when observing the spot rate, the CNY and the CNH rate only differ marginally.

However, when looking at the price of futures for longer maturity, there is a significant discrepancy (in the CNY/CNY case, up to 4% when corrected for maturity).

This is puzzling as the future face value follows the same principle as the present one.

In the present work we propose a continuous time equilibrium in two similar market which are scholastically coupled.

This solution of which is given by a coupled quadratic jump diffusion FBDE that provide an equilibrium price on both markets.

We then use a second equilibrium to price futures and therefore provide some interpretations as for the price discrepancy observed on the market.

This is a joint work with Xuan Tao, Peng Luo, Wang Tan and Wang Tao

## [04244] Portfolio Selection, Periodic Evaluations and Risk Taking

**Format :** Talk at Waseda University

**Author(s) :** Alex Sing-lam Tse (University College London)Harry Zheng (Imperial College London)

**Abstract :** We present a continuous-time portfolio selection problem faced by an agent with S-shaped preference who maximizes the utilities derived from the portfolio's periodic performance over an infinite horizon. The periodic reward structure creates subtle incentive distortion. In some cases, local risk aversion is induced which discourages the agent from risk taking in the extreme bad states of the world. In some other cases, eventual ruin of the portfolio is inevitable and the agent underinvests in the good states of the world to manipulate the basis of subsequent performance evaluations. We outline several important elements of incentive design to contain the long-term portfolio risk.

## [01070] PDE Based Image Processing

**Session Time & Room :**

01070 (1/2) : 4D (Aug.24, 15:30-17:10) @G502

01070 (2/2) : 4E (Aug.24, 17:40-19:20) @G502

**Type :** Proposal of Minisymposium

**Abstract :** Partial differential equation (PDE) method shows better performance than traditional image processing methods, and some new ideas have never been considered in traditional image processing, such as affine invariant feature extraction, image structure and texture decomposition, etc. This method aims to establish the mathematical model of a partial differential equation, and then make the image change according to the PDE, and finally achieve the desired effect. PDE models are mathematically robust and also provide insights in developing new algorithms. Fusion of AI/ML methods and PDE models makes it even more effective.

**Organizer(s) :** B. V. Rathish Kumar

**Classification :** 35G25

**Minisymposium Program :**

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01070 (1/2) : 4D @G502 [Chair: Prof. BVR Kumar]

## [01942] A new PDE model for Image Inpainting

**Format :** Online Talk on Zoom

**Author(s) :** Abdul Halim (King Abdullah University of Science and Technology)B.V. Rathish Kumar (IIT Kanpur)

**Abstract :** In this talk, I will present a fourth-order PDE model with a multi-well potential function for grayscale image inpainting. Convexity splitting in time and Fourier spectral method in space has been used to derive an unconditional scheme on time. The stable scheme is both consistent and convergent. Also, I present the fractional variant of the time discretized scheme by replacing the Laplacian with its fractional counterpart. Numerical results for some standard test images will be presented and will be compared with the results of other existing models in the literature. To quantify the quality of the recovered image, we calculate the image quality metric such as PSNR, SNR, and SSIM.

## [01962] Fractional Calculus Based Approach for Retinal Blood Vessel Segmentation

**Format :** Online Talk on Zoom

**Author(s) :** Rajesh Kumar Pandey (Indian Institute of Technology (BHU) Varanasi)Varun Makkar (Indian Institute of Technology (BHU) Varanasi)Rathish Kumar Venkatesulu Bayya (Indian Institute of Technology Kanpur)

**Abstract :** We will discuss a new fractional filter and an algorithm for retinal blood vessel segmentation. The proposed fractional filter is designed with the help of a weighted fractional derivative and an exponential weight factor. Firstly, the image is denoised using developed fractional. Then, multi-scale line detector is used to compute

the line responses at multiple lengths using a punctured window of fixed dimensions. The final response is the computed as the arithmetic mean of all responses at different scales and the underlying image intensity. This enhances the retinal blood vessels and suppresses rest of the background. Finally, hysteresis thresholding is applied to obtain the segmented vessels. Experiments are performed on two well-studied evaluation databases named STARE and DRIVE and the simulation results are discussed.

## [02860] Game theoretic Approach for Image segmentation and Image restoration by using Fractional PDE

**Format :** Online Talk on Zoom

**Author(s) :** Kedarnath Buda (Indian Institute of Technology Kanpur, India) Rathish Kumar Venkatesulu Bayya (Indian Institute of Technology Kanpur)

**Abstract :** In this study, a game theoretic algorithm through which a noisy image is both restored and segmented simultaneously is proposed. We define a two cost functions for two players of a Game. One player is Image restoration and another one is Image segmentation. Both of them are further constrained by fractional PDEs. The establish the Nash equilibrium for this game, which is an ideal strategy for deciding the amount of image restoration and image segmentation that can be done through the optimization of the bi-objective cost functions. We then numerically compute this with some real images.

## [02862] Higher Order PDE Model for Effective Image Denoising

**Format :** Talk at Waseda University

**Author(s) :** Rathish Kumar Venkatesulu Bayya (Indian Institute of Technology Kanpur) Abdul Halim (KAUST)

**Abstract :** In this talk we will introduce a new higher order nonlinear PDE model for image denoising and demonstrate its ability to denoise without any staircase effect as routinely noticed with lower order PDE models. We use convexity splitting based Fourier Spectral scheme for the computation of the denoised version of a given noisy image. Fourier spectral method is both accurate and faster than many standard approaches. Performance of the model and the method will be discussed based on the benchmark test images and the related computational metrics.

01070 (2/2) : 4E @G502 [Chair: Prof. BVR Kumar]

## [02870] A Framework for Motion Estimation with Physics-Based Constraints in Image Sequences

**Format :** Online Talk on Zoom

**Author(s) :** Hirak Doshi (Doctoral Research Scholar) Uday Kiran Nori (Associate Professor)

**Abstract :** Motion estimation using variational models has been a central topic in mathematical image processing for many years. The Horn and Schunck model's variational approach to optical flow motion estimation is a seminal work that has been studied in-depth to develop different variational models for motion estimation. However, the Horn and Schunck model's constancy assumption cannot reflect the reality of actual motion, as deformation effects of fluid, illumination variations, perspective changes, poor contrast, etc., directly affect the important motion parameters. Therefore, physics-dependent motion estimation algorithms have been extensively investigated in the literature.

In this paper, we propose a generic framework that captures physics-based constraints for motion estimation as perceived at the smallest intensity level (pixel) of an image sequence. These constraints are introduced as non-conservative terms that capture the loss of particles at the pixel-level, in the minimizing energy functional. We demonstrate our framework with two physics-based constraints, the continuity constraint for fluid motion and the harmonic constraint for capturing rotation in the images. Furthermore, we theoretically justify the effectiveness of our model through the techniques of Augmented Lagrangian and maximal monotone operators.

We establish the mathematical well-posedness of the associated PDE in the Hilbert space setting. For the linear case, we perform a decoupling of the associated PDE into diffusion equations on the curl and divergence of the flow field through a diagonalization with the Cauchy-Riemann operator. This decoupling process suggests that our approach preserves the spatial characteristics of the divergence and the vorticities of the flow field.

We adapt the first-order primal-dual Chambolle-Pock algorithm to obtain the minimization of our variational problem. We demonstrate the robustness of our approach through velocity plots and use the Average Angular Error (AAE) and End-Point Error (EPE) as performance metrics. We test our algorithm on several relevant datasets and show good results. In particular, for the Middlebury dataset, we show that our algorithm outperforms some of the state-of-the-art Horn and Schunk based flow models.

Moreover, for the fluid motion estimation case, a primal-dual implementation of our two-phase refinement model has a faster convergence rate of  $O(1/N)$  compared to the  $O(1/\sqrt{N})$  convergence rate of a direct primal-dual implementation of the Liu-Shen continuity-based model, where  $N$  is the number of iterations. Although we do not have a theoretical proof for this observed efficiency, we provide substantial empirical evidence.

## [03393] On the convergence analysis of DNN for vorticity stream function formulation and application

**Format :** Online Talk on Zoom

**Author(s) :** Rajendra Kumar (Student) Rathish Kumar Venkatesulu Bayya (Indian Institute of Technology Kanpur) Ming-Chih Lai (National Yang Ming Chiao Tung University, Taiwan)

**Abstract :** The physics-informed neural network is a completely mesh-free method for partial differential equations. In this paper, We introduce a Physics-informed neural network for the two dimensions Navier-stokes equation in the vorticity-stream function form with boundary conditions. We estimate the error of the physics-informed neural network for vorticity stream function formulation and theoretically establish the convergence of the computational procedure. In Deep neural network representation imposing the boundary condition is one of the main issues. We successfully incorporate periodic boundary conditions in the vorticity stream function formulation which is known for its difficulty in training the model. We have successfully applied PINNs on applications such as the Double shear layer and Taylor vortex problem

## [01071] Recent Advances on Groebner Bases and Their Applications

**Session Time & Room :**

01071 (1/2) : 2C (Aug.22, 13:20-15:00) @G305

01071 (2/2) : 2D (Aug.22, 15:30-17:10) @G305

**Type :** Proposal of Minisymposium

**Abstract :** The purpose of this mini-symposium is to share recent developments in the theory of Gr"obner bases and their applications. Gr"obner bases have been studied by many researchers and have been used in various fields including commutative algebra, algebraic geometry, and engineering. Solving interesting open problems and devising efficient algorithms are still highly desired. In this mini-symposium, we will discuss, in particular, the complexity of Gr"obner basis computation, applications of Gr"obner bases, and algorithms for Gr"obner bases in parametric, non-commutative, or valuation polynomial rings.

**Organizer(s) :** Yuki Ishihara

**Classification :** 13Pxx, 14Qxx, 68W30

**Minisymposium Program :**

01071 (1/2) : 2C @G305 [Chair: Yuta Kambe]

## [01758] Parametric Ideal Operations

**Format :** Talk at Waseda University

**Author(s) :** Yuki Ishihara (Tokyo University of Science)

**Abstract :** We present several algorithms for parametric ideal operations of polynomial ideals. Let  $K[X] = K[x_1, \dots, x_n]$  be the polynomial ring over a field  $K$  and  $K[A, X]$  the parametric polynomial ring with parameters  $A = \{a_1, \dots, a_m\}$ . Let  $\varphi_\alpha$  be the homomorphism from  $K[A, X]$  to  $K[X]$  by  $\varphi_\alpha(f(A, X)) = f(\alpha, X)$  for  $\alpha \in K^m$ . For an ideal operation  $F$  and parametric ideals  $I_1, \dots, I_r$ , we compute a set of pairs  $\{(A_i, G_i)\}_{i=1}^s$  s.t.  $\bigcup_{i=1}^s A_i = K^m$  and  $\varphi_\alpha(G_i)$  is a Groebner basis of  $F(\varphi_\alpha(I_1), \dots, \varphi_\alpha(I_r))$  for any  $\alpha \in A_i$ .

## [01892] On the complexity of Groebner basis computation

**Format :** Talk at Waseda University

**Author(s) :** Kazuhiro Yokoyama (Rikkyo University)

**Abstract :** The complexity of computation of Groebner basis is heavily related to the syzygy of given generating set. We will discuss this relation for generic case, where coefficients of generating set can be considered as parameters.

## [01851] On Parametric Border Basis and Comprehensive Gröbner System

**Format :** Talk at Waseda University

**Author(s) :** Yosuke Sato (Tokyo University of Science)

**Abstract :** A border basis is an alternative tool to a Gröbner basis for handling a polynomial ideal.

One of the most important properties of a border basis is its stability.

Though this property is cited by many researchers,

its precise definition has not been given anywhere yet.

We give its rigorous definition in terms of a parametric polynomial ideal and introduce several properties which enable us to have a simple representation of a parametric polynomial ideal.

## [01843] Universal Analytic Gröbner bases, Tate Algebras and toward Tropical Analytic Geometry

**Format :** Talk at Waseda University

**Author(s) :** Tristan Vaccon (Limoges University)Thibaut Verron (Johannes Kepler University)

**Abstract :** Tate algebras are defined as multivariate formal power series over a  $p$ -adic field, with a convergence condition.

We will present the concept of Universal Analytic Gröbner Basis for a polynomial ideal:

a finite polynomial basis of an ideal such that it is a Gröbner basis in any of the completions into Tate algebras for any (rational) convergence radius.

We will present how to compute it and its relation with tropical varieties.

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01071 (2/2) : 2D @G305 [Chair: Yuki Ishihara]

## [01891] Criteria for Grobner bases and degenerations by structure of signatures

**Format :** Talk at Waseda University

**Author(s) :** Yuta Kambe (Mitsubishi Electric Corporation)

**Abstract :** The F5 algorithm was presented by Faugere in 2002 and variants of the F5 algorithm have been proposed by various researchers called signature based algorithms (SBAs). The concept of signatures was revised by Arri-Perry in 2011 as normal monomials for syzygies and Vaccon-Yokoyama presented an implementable SBA in 2017 with the concept of guessed signatures. The speaker will talk about these new concepts and his new criterion theorem for Grobner bases and degenerations.

## [01876] On signature-based algorithm for tropical Groebner bases on Weyl algebra

**Format :** Talk at Waseda University

**Author(s) :** Ari Dwi Hartanto (Department of Mathematics, Universitas Gadjah Mada)Katsuyoshi Ohara (Faculty of Mathematics and Physics, Kanazawa University)

**Abstract :** The computational aspect of tropical Groebner basis for polynomial rings introduced by A.W.Chan is extended to the Weyl algebras over fields with valuations. A term order with valuation is designed to be a generalization of the tropical term orders studied by A.W.Chan and by T.Vaccon. Although it is not well-ordering, a signature-based algorithm can still be developed. The minimal natural signature of a polynomial exists. The F5 criterion is then adopted for this context.

## [01898] Algorithms for bivariate lexicographic Groebner bases

**Format :** Talk at Waseda University

**Author(s) :** Xavier DAHAN (Tohoku University)

**Abstract :** The lexicographic monomial order for Groebner bases is fundamental since it holds the elimination property. This also implies strong structural properties, as shown by Lazard in 1985 in the case of two variables. Yet these properties have not been fully exploited. I will explain how they allow to perform Chinese Remainder Theorem like operations in several situations, as well as the difficulties in remaining cases. I will also discuss extensions to more than two variables.

## [01885] An algebraic approach to factor analysis

**Format :** Talk at Waseda University

**Author(s) :** Ryoya Fukasaku (Kyushu University)Kei Hirose (Kyushu University)Yutaro Kabata (Nagasaki University)Keisuke Teramoto (Hiroshima University)

**Abstract :** When the maximum likelihood method is used in factor analysis, it is not uncommon for an unique variance less than or equal to zero to be generated, which is known as the improper solution problem. Although numerical approaches have been made to this problem, algebraic approaches have not. Therefore, we aim to exactly describe the solution space associated with the maximum likelihood method in factor analysis by making use of computational algebraic methods such as Gröbner bases and cylindrical algebraic decomposition.

# [01072] Data-Driven Methods in Scientific Machine Learning

**Session Time & Room :**

01072 (1/2) : 4D (Aug.24, 15:30-17:10) @E803

01072 (2/2) : 4E (Aug.24, 17:40-19:20) @E803

**Type :** Proposal of Minisymposium

**Abstract :** The ample availability of data for scientific problems, in addition to developments in hardware and software for machine and deep learning have changed the way mathematicians approach problems, particularly those in numerical analysis and scientific computing. Rather than relying strictly on the physics of the problem at hand for modeling and computing, data-driven methods incorporate observational data to inform their solutions. This session focuses on significant advances in data-driven methods and machine learning for a variety of problems in scientific computing, including but not limited to: function approximation, inverse problems, dynamical systems, dimensionality reduction, and generally scientific machine learning.

**Organizer(s) :** Victor Churchill, Dongbin Xiu

**Classification :** 65Z05, 62R07, 68T07, 68T09, Scientific Machine Learning

**Minisymposium Program :**

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01072 (1/2) : 4D @E803 [Chair: Victor Churchill]

## [05116] Acceleration of multiscale solvers via adjoint operator learning

**Format :** Talk at Waseda University

**Author(s) :** Emanuel Eld Ström (KTH Royal Institute of Technology)Ozan Öktem (KTH Royal Institute of Technology)Anna-Karin Tornberg (KTH Royal Institute of Technology)

**Abstract :** We leverage recent advances in operator learning to accelerate multiscale solvers for laminar fluid flow over a rough boundary. We focus on the HMM method, which involves formulating the problem through a coupled system of microscopic and macroscopic subproblems. Solving microscopic problems can be viewed as a nonlinear operator mapping from the space of micro domains to the solution space. Our main contribution is to use an FNO-type architecture to perform this mapping.

**[05635] A Stochastic MaxiIn this work, we introduce a stochastic maximum principle (SMP) approach for solving the reinforcement learning problem with the assumption that the unknmum Principle Approach for Reinforcement Learning with Parameterized Environment**

**Format :** Talk at Waseda University

**Author(s) :** Feng Bao (Florida State University)Richard Archibald (Oak Ridge National Lab)Jiongmin Yong (University of Central Florida)

**Abstract :** In this work, we introduce a stochastic maximum principle (SMP) approach for solving the reinforcement learning problem with the assumption that the unknowns in the environment can be parameterized based on physics knowledge. For the development of numerical algorithms, we apply an effective online parameter estimation method as our exploration technique to estimate the environment parameter during the training procedure, and the exploitation for the optimal policy is achieved by an efficient backward action learning method for policy improvement under the SMP framework. Numerical experiments are presented to demonstrate that the SMP approach for reinforcement learning can produce reliable control policy, and the gradient descent type optimization in the SMP solver requires less training episodes compared with the standard dynamic programming principle based methods.

**[05649] A pseudo-reversible normalizing flow for stochastic dynamical systems with various initial distributions**

**Format :** Talk at Waseda University

**Author(s) :** Guannan Zhang (Oak Ridge National Laboratory)

**Abstract :** We present a pseudo-reversible normalizing flow method for efficiently generating samples of the state of a stochastic differential equation (SDE) with various initial distributions. The primary objective is to construct an accurate and efficient sampler that can be used as a surrogate model for computationally expensive numerical integration of SDE, such as those employed in particle simulation. After training, the normalizing flow model can directly generate samples of the SDE's final state without simulating trajectories. Existing normalizing flow model for SDEs depend on the initial distribution, meaning the model needs to be re-trained when the initial distribution changes. The main novelty of our normalizing flow model is that it can learn the conditional distribution of the state, i.e., the distribution of the final state conditional on any initial state, such that the model only needs to be trained once and the trained model can be used to handle various initial distributions. This feature can provide a significant computational saving in studies of how the final state varies with the initial distribution. Additionally, we propose to use a pseudo-reversible network architecture to define the normalizing flow model, which has sufficient expressive power and training efficiency for a variety of SDEs in science and engineering, e.g., in particle physics. We provide a rigorous convergence analysis of the pseudo-reversible normalizing flow model to the target probability density function in the Kullback–Leibler divergence metric. Numerical experiments are provided to demonstrate the effectiveness of the proposed normalizing flow model.

01072 (2/2) : 4E @E803 [Chair: Victor Churchill]

**[05632] Flow Map Learning for Unknown Dynamical Systems: Overview, Implementation, and Benchmarks**

**Format :** Talk at Waseda University

**Author(s) :** Victor Churchill (Trinity College)Dongbin Xiu (The Ohio State University)

**Abstract :** Flow map learning has shown promise for data-driven modeling of unknown dynamical systems. A remarkable feature is the capability of producing accurate predictive models for partially observed systems, even when their exact mathematical models do not exist. We present an overview of the framework, as well as the important computational details for its successful implementation. A set of well defined benchmark problems are presented in full numerical detail to ensure accessibility for cross-examination and reproducibility.

# [01074] Approximation Theory, Approximation Methods and Applications (ATAMA)

**Session Time & Room :**

01074 (1/3) : 5B (Aug.25, 10:40-12:20) @F310

01074 (2/3) : 5C (Aug.25, 13:20-15:00) @F310

01074 (3/3) : 5D (Aug.25, 15:30-17:10) @F310

**Type :** Proposal of Minisymposium

**Abstract :** Approximation theory is a subject that serves as an important bridge between pure and applied mathematics. It has become a very important branch of mathematics and is of fundamental support of many new disciplines and research areas.

The proposed minisymposium aims to merge together active researchers in the following topics:  
polynomial inequalities in the multivariate real and complex fields, pluripotential numerics, kernel-based approximation, generalized sampling type operators and exponential sampling.

Special attention will be given to applications, modeling, as well as computational and numerical aspects in approximation.

**Organizer(s) :** Leokadia Bialas-Ciez, Stefano De Marchi

**Classification :** 41Axx, 65Dxx, 42A10

**Minisymposium Program :**

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01074 (1/3) : 5B @F310 [Chair: Leokadia Bialas-Ciez]

## [04256] Approximation Theory, Approximation Methods and Applications: an introduction

**Format :** Online Talk on Zoom

**Author(s) :** Stefano De Marchi (University of Padova)

**Abstract :** In this initial talk, I will briefly summarize why we have proposed such a mini-symposium, why approximation theory is still an important research subject for numerical and analytical analysts, and why approximation theory can help industrial applications. I will also outline the main contributions provided by all the speakers invited to this mini-symposium.

## [04857] On the quality of adaptive methods for numerical approximation

**Format :** Talk at Waseda University

**Author(s) :** Leszek Plaskota (University of Warsaw)

**Abstract :** Methods for numerical approximation generally fall into two categories:  
nonadaptive algorithms and adaptive algorithms. By ‘adaptive’ we mean that  
in its successive steps the algorithm uses information about the underlying function  
obtained from the previous steps. If the function possesses some singularities and  
is otherwise smooth, then adaption is necessary to restore the right convergence rate.  
For globally smooth functions adaptive algorithms can essentially lower asymptotic constants.  
We present recent quantitative results on the subject.

## [05019] Monte Carlo approximation of non-autonomous Julia sets

**Format :** Online Talk on Zoom

**Author(s) :** Maciej Klimek (Uppsala University)

**Abstract :** In the metric space of compact, pluriregular and polynomially convex subsets of  $\mathbb{C}^N$ , both finite and infinite families of proper polynomial mappings generate a variety of Julia type compact sets, known also as the composite Julia sets.

These sets can be interpreted as attractors of generalized iterated function systems. Since stochastic approximation of composite Julia sets is viable, some of those sets can be visualized with the help of Monte Carlo methods.

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01074 (2/3) : 5C @F310 [Chair: Elisabeth Larsson]

## [05151] Projection Constants for Spaces of Multivariate Polynomials

**Format :** Online Talk on Zoom

**Author(s) :** Mieczysław Mastyło (Adam Mickiewicz University, Poznań)

**Abstract :** We study the projection constant of spaces of polynomials with the supremum norm over the unit ball of finite dimensional Banach sequence space including the Hilbert space. We consider the action of topological groups over these spaces of polynomials and provide some integral formulas for their projection constants. This cycle of ideas leads to the asymptotic behaviour of the projection constants of spaces of Dirichlet polynomials and the space of nuclear operators on  $\ell_2^n$ .

## [05170] Stable high-order randomized cubatures for integration in arbitrary dimension

**Format :** Online Talk on Zoom

**Author(s) :** Giovanni Migliorati (Sorbonne Université)

**Abstract :** We present cubature formulae for the integration of functions in arbitrary dimension and arbitrary domain. These cubatures are exact on a given finite-dimensional subspace  $V_n$  of  $L^2$  of dimension  $n$ , they are stable with high probability and are constructed using  $m$  pointwise evaluations of the integrand function with  $m$  proportional to  $n \log n$ . For these cubatures we provide a convergence analysis showing that the expected cubature error decays as  $m^{-1/2}$  times the  $L^2$  best approximation of the integrand function in  $V_n$ .

## [05108] On empirical adequacy of approximations within mathematical models

**Format :** Online Talk on Zoom

**Author(s) :** Michael A Slawinski (Memorial University)

**Abstract :** We discuss a phenomenological model formulated to study the power applied by a cyclist on a velodrome.

The dissipative forces we consider are air resistance, rolling resistance, lateral friction and drivetrain resistance.

Also, the power is used to increase the kinetic and potential energy.

Following derivations and justifications of expressions that constitute this mathematical model, we discuss them in the context of measurements.

## [05186] On technical considerations of velodrome track design

**Format :** Online Talk on Zoom

**Author(s) :** Theodore Stanev (Memorial University of Newfoundland)

**Abstract :** We present a novel approach to velodrome track design. The mathematical model uses differential geometry to form a three-dimensional ruled surface. The track is comprised of straight lines, the arcs of circles, and connecting transition curves, whose features are derived from the Frenet-Serret relations. Symmetric and asymmetric designs are obtained using least-squares optimization. The formulation may be used to design velodrome tracks of a wide variety of track geometry specifications.

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01074 (3/3) : 5D @F310 [Chair: Stefano De Marchi]

## [05085] Optimal scaling of radial basis function approximations

**Format :** Talk at Waseda University

**Author(s) :** Elisabeth Larsson (Uppsala University) Boštjan Mavrič (Institute of Metals and Technology) Andreas Michael (Uppsala University) Ulrika Sundin (Uppsala University)

**Abstract :** We revisit the question about which shape parameter to use in radial basis function approximations. We compute the flat shape parameter limit of a Gaussian interpolant as an expansion in even powers of the shape parameter and illustrate how the correction terms cancel the dominant part of the error for smooth solution

functions. We also provide a closed form expression that explains the shape of the error curves in terms of the shape parameter.

### [04984] Interpolation on the sphere using series kernels

**Format :** Online Talk on Zoom

**Author(s) :** Janin Jäger (KU Eichstätt-Ingolstadt) Simon Hubbert (Birkbeck University of London)

**Abstract :** We study the use of series kernels for interpolation and approximation of data on a d-dimensional sphere. Kernels in series representation allow us to easily deduce geometric properties of the kernel, strict positive definiteness of the kernel, smoothness of the approximant and approximation error estimates. We will show how series representations can be derived for restrictions of radial basis functions from the surrounding Euclidean space to the sphere and state the explicit expansion for the generalised Wendland functions.

### [05064] $(\beta, \gamma)$ -Chebyshev functions and points

**Format :** Online Talk on Zoom

**Author(s) :** Francesco Marchetti (University of Padova)

**Abstract :**  $(\beta, \gamma)$ -Chebyshev functions are a generalization of classical Chebyshev polynomials of the first kind. They consist of a family of orthogonal functions on a subset of  $[-1, 1]$ , which indeed satisfies a three-term recurrence formula and complies with various properties of classical families of orthogonal polynomials. Moreover, for certain configurations of parameters  $\beta$  and  $\gamma$ , the roots of  $(\beta, \gamma)$ -Chebyshev functions contained in the corresponding orthogonality interval lead to a stable polynomial interpolation process.

## [01077] Recent Advances on Spectral Methods and Applications

**Session Time & Room :**

01077 (1/2) : 5B (Aug.25, 10:40-12:20) @E709

01077 (2/2) : 5C (Aug.25, 13:20-15:00) @E709

**Type :** Proposal of Minisymposium

**Abstract :** During the past several years, significant progress has been made in spectral methods and applications, especially in challenge problems such as numerical approximations for non-local and high-dimensional partial differential equations, where spectral and high-order methods are often preferred to low-order methods due to high-accuracy and lower memory request. This minisymposium aims to bring together active researchers in related areas to present and discuss their newest advances in both mathematical theory and numerical algorithms of efficient spectral numerical approximations for challenge scientific and engineering applications.

**Organizer(s) :** Hui-Yuan Li (Institute of Software Chinese Academy of Sciences), Li-Lian Wang (Nanyang Technological University), Haijun Yu

**Classification :** 65N35, 65M70

**Minisymposium Program :**

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01077 (1/2) : 5B @E709 [Chair: Li-Lian Wang]

### [04186] A positive and moment-preserving Fourier spectral method

**Format :** Talk at Waseda University

**Author(s) :** Zhenning Cai (National University of Singapore) Bo Lin (National University of Singapore)

**Abstract :** We present a novel Fourier spectral method that utilizes optimization techniques to ensure the positivity and conservation of moments in the space of trigonometric polynomials. We rigorously analyze the accuracy of the new method and prove that it maintains spectral accuracy. To solve the optimization problem, we propose an efficient Newton solver that has quadratic convergence rate. Applications to the Boltzmann equation are considered in our numerical tests.

## [03237] Efficient structure-preserving spectral methods for plasma simulations

**Format :** Talk at Waseda University

**Author(s) :** Zhiguo Yang (Shanghai Jiao Tong University)

**Abstract :** In this talk, we present  $H^1$ -,  $H(\text{div})$  and  $H(\text{curl})$ -conforming spectral method with exact preservation of the curl/divergence-free constraints for two typical PDEs arising from plasma simulations. One is the incompressible visco-resistive MHD system and the other one is the Vlasov-Ampere system. Two key ingredients, i.e. exact de Rham complexes and their commuting diagram, and the derivative property of the generalized Jacobi polynomials, are essential for the derivation of the desired basis functions. Besides, we propose a novel efficient solution algorithm based on simultaneous multiple-matrices diagonalisation technique. Ample 2D and 3D numerical examples illustrate both the accuracy and efficiency of the proposed methods.

## [04790] A deep adaptive sampling method for the approximation of PDEs

**Format :** Talk at Waseda University

**Author(s) :** Kejun Tang (Changsha Institute for Computing and Digital Economy, Peking University) Jiayu Zhai (ShanghaiTech University) Xiaoliang Wan (Louisiana State University)

**Abstract :** In this work, we develop an adaptive sampling strategy when approximating the PDE solution with a neural network. Two neural networks will be trained simultaneously through a min-max optimization problem, which is formulated by coupling PINN and the optimal transport. One neural network is used as a surrogate model of the true solution and the other neural network is used to optimize the collocation points in the training set. Numerical experiments will be presented.

## [04098] A variable time-step scheme for Navier-Stokes equations

**Format :** Talk at Waseda University

**Author(s) :** Yana DI (Beijing Normal University)

**Abstract :** In the talk, the implicit-explicit (IMEX) second-order backward difference (BDF2) scalar auxiliary variable (SAV) scheme for Navier-Stokes equation with periodic boundary conditions (*Huang and Shen, SIAM J. Numer. Anal.*, 2021) has been generalized to a variable time-step IMEX-BDF2 SAV scheme. We derive global and local optimal  $H^1$  error estimates in 2D and 3D, respectively. An adaptive time-stepping strategy has also been designed and numerical examples will confirm the effectiveness and efficiency of our proposed methods.

01077 (2/2) : 5C @E709 [Chair: Hui-Yuan Li]

## [03896] Barycentric Interpolation Based on Equilibrium Potential

**Format :** Talk at Waseda University

**Author(s) :** Shuhuang Xiang (Central South University) Kelong Zhao (Central South University)

**Abstract :** A novel barycentric interpolation algorithm with specific exponential convergence rate is designed for analytic functions defined on the complex plane, with singularities located near the interpolation region, where the region is compact and can be disconnected or multiconnected. The core of the method is the efficient computation of the interpolation nodes and poles using discrete distributions that approximate the equilibrium logarithmic potential, achieved by solving a Symm's integral equation. It takes different strategies to distribute the poles for isolated singularities and branch points, respectively. In particular, if poles are not considered, it derives a polynomial interpolation with exponential convergence. Numerical experiments illustrate the superior performance of the proposed method.

## [04757] Log orthogonal functions in semi-infinite intervals: approximation results and applications

**Format :** Talk at Waseda University

**Author(s) :** Sheng Chen (Beijing Normal University at Zhuhai)

**Abstract :** We construct two new classes of log orthogonal functions in semi-infinite intervals, log orthogonal functions (LOFs-II) and generalized log orthogonal functions (GLOFs-II), by applying a suitable log mapping to Laguerre polynomials. We develop a basic approximation theory for these new orthogonal functions and show that they can provide uniformly good exponential convergence rates for problems in semi-infinite intervals with slow decay at infinity. We apply them to solve several linear and nonlinear differential equations whose solutions decay

algebraically or exponentially with very slow rates and present ample numerical results to show the effectiveness of the approximations by LOFs-II and GLOFs-II.

## [05466] A class of efficient spectral methods and error analysis for nonlinear Hamiltonian systems

**Format :** Online Talk on Zoom

**Author(s) :** Waixiang Cao (Beijing Normal University )Jing An (Guizhou Normal university)Zhimin Zhang (Wayne state University )

**Abstract :** In this talk, we investigate efficient numerical methods for nonlinear Hamiltonian systems. Three polynomial spectral methods (including spectral Galerkin, Petrov-Galerkin, and collocation methods) coupled with domain decomposition are presented and analyzed. Our main results include the energy and symplectic structure-preserving properties and error estimates. We prove that the spectral Petrov-Galerkin method preserves the energy exactly while both the spectral Gauss collocation and spectral Galerkin methods are energy conserving up to spectral accuracy. While it is well known that collocation at Gauss points preserves symplectic structure, we prove that the Petrov-Galerkin method preserves the symplectic structure up to a Gauss numerical quadrature error and the spectral Galerkin method preserves the symplectic structure up to spectral accuracy error. Finally, we show that all three methods converge exponentially, which makes it possible to simulate the long time behavior of the system. Numerical experiments indicate that our algorithms are efficient.

## [01081] New Trends in Education of Applied Mathematics, Industry, Technology and Knowledge Transfer

**Session Time & Room :** 1E (Aug.21, 17:40-19:20) @A208

**Type :** Proposal of Minisymposium

**Abstract :** The field of applied mathematics is constantly evolving and it is important for professionals in the industry and academics to stay up-to-date with the latest trends and developments. This minisymposium is aimed at discussing how the recent technology developments are changing both how and what we need to teach in undergraduate applied mathematics programs. We will provide a platform for experts to share their insights and experiences on the current and future trends in the education of Applied Mathematics and its applications in industry and technology.

**Organizer(s) :** Dae-Jin Lee (IE University), David Gómez-Ullate (IE University), Luis Vega (UPV/EHU-BCAM)

**Classification :** 97M10, 97M20, 97D99, Mathematics and Education

**Minisymposium Program :**

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01081 (1/1) : 1E @A208

## [02936] Applied Mathematics curriculum in the 21 st century

**Author(s) :** Beatriz Rumbos (Instituto Tecnológico Autónomo de México)

**Abstract :** Throughout history, Mathematics has made it possible for humans to cope and understand their surroundings and to make our lives more predictable. In the 20th century, mathematical models became indispensable tools for the development of almost every discipline; thus, promoting the creation of Applied Mathematics degrees at universities worldwide. The essence of an Applied Mathematics undergraduate program is to endow the student with the knowledge and analytical skills, needed to model and solve problems arising in a diversity of fields. The complexity of modern societies, the boom of the knowledge economy, the pace of technological change and the increasing social responsibility of modern youth, call for a major overhaul in the Applied Mathematics curricula and its teaching methods. In this talk I shall address the actions that we have taken at ITAM in order to address these challenges.

## [01931] An innovative experience in a Computer Engineering programme

**Author(s)** : M. Teresa T. Monteiro (Centre Algoritmi, Systems and Production Department, University of Minho) Gabriel Hornink (Educational Media Laboratory, Department of Biochemistry, Institute of Biomedical Sciences, Federal University of Alfenas) Flávia Vieira (Centro de Investigação em Educação (CIEd), Institute of Education, University of Minho, Braga)

**Abstract** : The talk reports an innovative learner-centred experience developed with 146 graduate students in the course “Numerical Methods and NonLinear Optimization” in a Computer Engineering programme at the University of Minho, Portugal. Students developed collaborative MATLAB projects by applying a course topic to a real-world phenomenon. Project analysis and students’ perceptions collected through a survey showed that they became pro-active learners and developed their ability to formulate, analyse and solve problems from a multidisciplinary perspective.

## [04341] How the last few years have reshaped teaching First-Year mathematics

**Author(s)** : Joshua Jordan Capel (UNSW, School of Mathematics and Statistics)

**Abstract** : In this talk we will discuss how the past few years have reshaped the teaching of mathematics in the School of Mathematics and Statistics, UNSW (University of New South Wales) Sydney, Australia. We will discuss how the in-term and end-of-term assessment have been re-designed to scaffold student learning throughout term and test understanding instead of just rewarding rote learning and computing. We will also discuss how this style has been embraced or challenged by university administrators and accreditation bodies, and speculate on what future challenges await us.

## [04591] Experiencing Mathematics: Compute. Intuit. Imagine. Create.

**Author(s)** : Amrik Sen (Plaksha University)

**Abstract** : If the next generation of engineering and science students are to be trained with the skills required to address contemporary societal and environmental challenges then both the curriculum and pedagogy of mathematics needs to be re-visited. I propose that training students to use computer technology to do mathematics and incorporating experiential projects as an immersive learning technique will foster intuition and imagination necessary to anchor abstract conceptual learnings to practical applications.

## [01088] Differential Equations meet Data: Scientific Machine Learning for Cardiovascular Applications

**Session Time & Room :**

01088 (1/4) : 3E (Aug.23, 17:40-19:20) @E708

01088 (2/4) : 4C (Aug.24, 13:20-15:00) @E708

01088 (3/4) : 4D (Aug.24, 15:30-17:10) @E708

01088 (4/4) : 4E (Aug.24, 17:40-19:20) @E708

**Type** : Proposal of Minisymposium

**Abstract** : In silico models offer effective tools to address cardiovascular diseases and quantitatively analyze clinical data. Recently, many methods have been proposed to blend numerical solvers with machine learning techniques. These approaches hold promise for the patient-specific personalization of models and for the acceleration of their numerical resolution. This minisymposium will offer a forum to discuss the state-of-the-art and future lines of research toward an increasingly effective integration between clinical data and numerical simulations

**Organizer(s)** : Francesco Regazzoni, Stefano Pagani, Francisco Sahli Costabal, Simone Pezzuto

**Classification** : 65Mxx, 65Zxx

**Minisymposium Program** :

01088 (1/4) : 3E @E708 [Chair: Simone Pezzuto]

## [04634] Scientific machine learning approaches for many-query problems in cardiovascular applications

**Format :** Online Talk on Zoom

**Author(s) :** Stefano Pagani (MOX, Department of Mathematics, Politecnico di Milano)Francesco Regazzoni (MOX, Dipartimento di Matematica, Politecnico di Milano)Luca Dede' (Politecnico di Milano)Alfio Quarteroni (Politecnico di Milano, EPFL)

**Abstract :** In many cardiovascular applications, only partial and (possibly) noisy measurements of the phenomenon are available, limiting data-driven techniques in robustly reconstructing quantities of interest. Scientific machine learning approaches compensate for this partial information by integrating physics-based parametric differential models into machine/deep learning models, enabling efficient and accurate solutions to inverse or parameter estimation problems. In this talk, we present some numerical examples of scientific machine learning strategies in computational medicine.

## [04639] GPU-Parallel Cardiac Simulation

**Format :** Talk at Waseda University

**Author(s) :** Toby Simpson (Università della Svizzera italiana)Rolf Krause (Università della Svizzera italiana)

**Abstract :** The computational cost of current approaches to whole heart simulation make them impractical for research or clinical application.

We compute a complete description of a human heartbeat, including electrophysiology, solid mechanics and fluid dynamics, on a single Graphics Processing Unit (GPU) within a few minutes.

The implementation via a matrix- and mesh-free Finite Volume discretisation, is simple enough to allow patient-specific fitting or provide ground truth data to machine learning algorithms.

## [05161] In-silico perivascular flow and transport

**Format :** Online Talk on Zoom

**Author(s) :** Marie Elisabeth Rognes (Simula Research Laboratory)

**Abstract :** Your brain has its own waterscape: whether you are reading, thinking or sleeping, fluid flows through or around the brain tissue, clearing waste in the process. These biophysical processes are crucial for the well-being and function of the brain. In spite of their importance we understand them but little. In this talk, I will give an overview of mathematical, mechanical and numerical approaches to gain new insight into mechanisms underlying brain clearance.

## [04430] Lipschitz Stabilised Autoencoders in Parameter Identification of Dynamical Systems

**Format :** Talk at Waseda University

**Author(s) :** Haibo Liu (Inria Paris)Damiano Lombardi (Inria Paris)Muriel Boulakia (Université de Versailles et Saint-Quentin en Yveline)

**Abstract :** The present work deals with data-driven modelling. Given a set of partial noisy observations of a dynamical system, we investigate using the Lipschitz stabilised auto-encoder to perform an intrinsic dimension estimation to understand how many parameters are responsible for the observed variability. By incorporating the information of the intrinsic dimensionality, we investigate a data-driven model that can complement the classical parameter identification method with the help of data.

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01088 (2/4) : 4C @E708 [Chair: Francesco Regazzoni]

## [05201] Accelerating hemodynamic predictions via machine learning

**Format :** Online Talk on Zoom

**Author(s) :** Noelia Grande Gutierrez (Carnegie Mellon University)

**Abstract :** Image-based computational blood flow simulations allow quantifying patient-specific hemodynamics with applications for personalized diagnosis, risk stratification, and treatment selection. However, the clinical translation of these methods is limited due to their high computational cost. We propose machine learning super-resolution to accelerate hemodynamic predictions. For upsampling simulation results, we combine physics-based

simulations on a coarse mesh with a graph neural network. Unstructured data (mesh) can be directly transformed into a graph representation, minimizing information loss.

## [04443] The fibrotic kernel signature: simulation-free prediction of atrial fibrillation

**Format :** Online Talk on Zoom

**Author(s) :** Francisco Sahli Costabal (Pontificia Universidad Católica de Chile)Simone Pezzuto (Università di Trento)Lia Gander (Università della Svizzera Italiana)Tomás Banduc (Pontificia Universidad Católica de Chile)

**Abstract :** We propose a fast classifier that is able to predict atrial fibrillation inducibility in patient-specific cardiac models. This is achieved by training the classifier on a variant of the Heat Kernel Signature, which includes information about the fibrosis. These features are fast to compute, when compared to standard cardiac models. The classifier is able to predict the inducibility of single points and also the overall inducibility of the model.

## [05176] Learning Reduced-Order Models for Blood Flow Simulations Using Graph Neural Networks

**Format :** Talk at Waseda University

**Author(s) :** Luca Pegolotti (Stanford University)Martin Pfaller (Stanford University)Natalia Rubio (Stanford University)Rita Brugarolas Brufau (Intel )Ke Ding (Intel)Eric Darve (Stanford University)Alison Marsden (Stanford University)

**Abstract :** We develop one-dimensional reduced-order models for simulating blood flow dynamics in complex cardiovascular geometries using a graph neural network trained on 3D hemodynamic data. Our method, which is a modified version of MeshGraphNet, accurately and efficiently predicts pressure and flow rate with errors below 2% and 3%, respectively, outperforming traditional physics-based models while maintaining high inference efficiency. Our findings demonstrate the potential of this approach in handling diverse anatomies and boundary conditions in physiological settings.

01088 (3/4) : 4D @E708 [Chair: Stefano Pagani]

## [04920] Fast and accurate reduced order modelling techniques for the simulation of blood flow dynamics

**Format :** Talk at Waseda University

**Author(s) :** Gianluigi Rozza (SISSA Trieste)

**Abstract :** Heart disease is one of the main cause of death worldwide, therefore in the last years the medical profession

has shown a growing attention for simulating blood flow dynamics through numerical methods.

The main purpose is to build a support for surgical procedure and to predict the progression of a disorder.

Full order mathematical models can be adopted for patient-specific cases, varying physical and geometrical parameters, however the complexity of the computational domain requires a fine discretization and as a result a considerable amount of time. Our works focus on the study of Reduced Order Models (ROMs), which are specifically formulated to reduce the computational cost of complex dynamics such as biomedical ones. A complete decoupling between an offline and an online stage is adopted to speed up high fidelity simulations, by splitting what can be done only once and what need to be evaluated for every new parameter to obtain a good ROM solution. Both intrusive and data-driven approaches are tested for patient-specific applications to investigate both the efficiency and the accuracy of the ROM framework.

## [04420] Parameter estimation in cardiac biomechanical models based on physics-informed neural networks

**Format :** Online Talk on Zoom

**Author(s) :** Federica Caforio (Institute of Mathematics and Scientific Computing, NAWI Graz, University of Graz)Francesco Regazzoni (MOX, Dipartimento di Matematica, Politecnico di Milan)Stefano Pagani (MOX, Department of Mathematics, Politecnico di Milano)Alfio Maria Quarteroni (MOX, Department of Mathematics, Politecnico di Milano)Gernot Plank (Gottfried Schatz Research Center: Division of Biophysics, Medical University of Graz)Gundolf Haase (Institute of Mathematics and Scientific Computing, NAWI Graz, University of Graz)

**Abstract :** In this talk a novel methodology is proposed, based on the integration of physics-informed neural networks methodologies with biophysically detailed three-dimensional cardiac biomechanical models, to generate robust and effective surrogate reduced-order models that are able to reconstruct displacement fields and locally

estimate heterogeneous passive mechanical properties. The accuracy and robustness of the proposed method are demonstrated in several benchmarks. This methodology potentially paves the way for the robust and effective identification of patient-specific physical properties.

## [03697] Super-resolution and denoising of 4D flow MRI via implicit neural representations

**Format :** Talk at Waseda University

**Author(s) :** Simone Saitta (Politecnico di Milano)Marcello Carioni (University of Twente)Subhadip Mukherjee (University of Bath)Carola-Bibiane Schönlieb (University of Cambridge)Alberto Redaelli (Politecnico di Milano)

**Abstract :** We trained sinusoidal representation networks (SIRENs) for denoising and super-resolution of time-varying 3-directional velocity fields measured in the aorta by 4D flow MRI. The performance of different SIREN architectures was evaluated on synthetic measurements and then we applied the best architecture to real 4D flow data of an aortic aneurysm. Our method provides a continuous representation of 4D velocity fields (super-resolution) and achieves denoising thanks to SIREN's spectral bias, outperforming state-of-the-art techniques.

01088 (4/4) : 4E @E708

## [01098] Elucidating theoretical biology and deep learning by algebraic statistics and topology

**Session Time & Room :** 1E (Aug.21, 17:40-19:20) @E504

**Type :** Proposal of Minisymposium

**Abstract :** Nonlinear algebra and topology are gaining popularity as a tool for studying theoretical biology including phylogenetics and mathematical neuroscience. Applying these modern mathematical fields can lead to a breakthrough in the important fields. However, there can be rather a limited access to the practical resources for the sophisticated mathematical methods. Thus, it is important to introduce the modern algebraic and topological methods and exchange their hands-on skills in person. In this minisymposium, each speaker will talk about the combinations of modern mathematical methods with statistical machine learning and their applications.

**Organizer(s) :** Keiji Miura

**Classification :** 62R01, 55-08, 68T07, 92D15

**Minisymposium Program :**

01098 (1/1) : 1E @E504 [Chair: Keiji Miura]

## [04921] Judging unlearnability from structures of deep neural networks for low dimensional inputs

**Format :** Talk at Waseda University

**Author(s) :** Keiji Miura (Kwansei Gakuin University)

**Abstract :** Zhang, Naitzat and Lim (2019) showed that a feedforward ReLU neural network is equivalent to a tropical rational map. Here we visualize the shapes of deep neural network functions by using the tropical algebra and judge its unlearnability of complicated boundaries. Especially, the limitation can be naturally interpreted by the tropical factorization of polynomials for the cases of one-dimensional input.

## [04805] Hit and Run Sampling from the Space of Phylogenetic Trees

**Format :** Talk at Waseda University

**Author(s) :** David Barnhill (Naval Postgraduate School)Ruriko Yoshida (Naval Postgraduate School)Keiji Miura (Kwansei Gakuin University)

**Abstract :** In this presentation we introduce a Markov Chain Monte Carlo (MCMC) Hit and Run (HAR) uniform sampler over a tropically convex space of ultrametrics. This is particularly important because by sampling from the space of ultrametrics, we are sampling from the space of phylogenetic trees, or tree space. This has wide ranging implications to statistical inference relating to drawing inference about the tree space. Specifically, we show how

part\_2

this HAR sampler can be employed to sample over the space of ultrametrics in order to non-parametrically estimate the phylogenetic tree distribution using what we call tropical density estimator (TDE) with the tropical metric. We compare the results of the TDE using the tropical metric against often used density estimation methods using the Billera-Holmes-Vogtman metric to show that TDE is more accurate and computationally less expensive.

## [04960] Approximate Computation of Vanishing Ideals

**Format :** Talk at Waseda University

**Author(s) :** Hiroshi Kera (Chiba University)

**Abstract :** The vanishing ideal of points is the set of all polynomials that vanish over the points. The approximate computation of generators has been developed at the intersection of computer algebra and machine learning in the last decade. Computer-algebraic algorithms have a rich theoretical background, whereas machine learning-oriented algorithms are designed for applications such as classification at the cost of some theoretical properties. This talk reviews the development of approximate computation of vanishing ideals.

## [01099] Physics-based and data-driven modeling for digital twins

**Session Time & Room :**

01099 (1/3) : 2C (Aug.22, 13:20-15:00) @A206

01099 (2/3) : 2D (Aug.22, 15:30-17:10) @A206

01099 (3/3) : 2E (Aug.22, 17:40-19:20) @A206

**Type :** Proposal of Minisymposium

**Abstract :** Digital twins have emerged in recent years as a paradigm for the lifetime operation of physical assets. A digital twin is an exact virtual representation of a physical asset that uses real-time data. The construction of a digital twin requires the use and sometimes union of different modeling methods that include physics-based modeling, data assimilation, data-driven modeling, and model reduction. This minisymposium has the goal to bring together researchers working on the theory and practice of modeling in the context of digital twins with a particular focus on industrial applications.

**Organizer(s) :** Karim Cherifi, Ion Victor Gosea

**Classification :** 93Axx, 93Cxx, 93-08

**Minisymposium Program :**

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01099 (1/3) : 2C @A206 [Chair: Ion Victor Gosea]

## [03242] Towards smart city digital twins

**Format :** Talk at Waseda University

**Author(s) :** Francisco Chinesta (ENSAM)Daniele Di Lorenzo (ESI)Victor Champaney (ENSAM)Angelo Pasquale (ENSAM)Amine Ammar (ENSAM)Elias Cueto (I3A)Dominique Baillargeat (CNRS@CREATE)

**Abstract :** Smart cities are composed of a number of coupled complex system of systems. Modelling them needs enhancing the traditional physics-based modelling approaches as well as speeding-up the predictions. Artificial intelligence and data-driven models obtained by using physics-informed and physics-augmented learning represents a valuable approach where accuracy and rapidity met. In this presentation advanced methodologies will be used for addressing complex scenarios, enabling real-time diagnosis and prognosis.

## [05203] Digital twins for green carbon processes

**Format :** Talk at Waseda University

**Author(s) :** Peter Benner (MPI for Dynamics of Complex Technical Systems, Magdeburg)Ion Victor Gosea (Max Planck Institute for Dynamics of Complex Technical Systems)

**Abstract :** Recent advances in scientific computing have made digital twins (DTs) increasingly popular in various fields,

including process engineering (ProcEng). DTs have the potential to transform ProcEng by enabling real-time monitoring or process optimization. However, their full potential in this area has yet to be realized. We provide an

overview of computational tools required for developing DTs in ProcEng. It characterizes models used to develop DTs and discusses the challenges and requirements associated with their implementation. We particularly focus on the development of sustainable chemical production processes in the context of a green carbon society.

## [01503] Hierarchical modeling of electrical machines in the context of digital twins

**Format :** Talk at Waseda University

**Author(s) :** Karim Cherifi (TU Berlin)Volker Mehrmann (TU Berlin)Philipp Schulze (TU Berlin)

**Abstract :** Digital twins of electrical machines require mathematical models that are accurate enough for the design and fast enough to be used for condition monitoring. This leads to a hierarchy of models that are used within the digital twin. These models must in addition incorporate the physical coupling between electrical, mechanical, and thermal phenomena for more accurate computations. In this talk, we present how one can construct this model hierarchy by incorporating physics-based and data-driven modeling.

## [04060] From physics to machine learning and back: Applications to fault diagnostics and prognostics

**Format :** Online Talk on Zoom

**Author(s) :** Olga Fink (EPFL)

**Abstract :** Deep learning requires representative data, but condition monitoring data for complex systems lack labels and representativeness. Integrating physics can help to overcome this.

The talk will give some insights into various techniques that combine physics-based and deep learning algorithms, as well as incorporate structural inductive bias for fault diagnostics and prognostics. The focus will be in particular on calibration-based hybrid approaches, physics-enhanced graph neural networks and on transformer-based architectures combined with transfer learning.

01099 (2/3) : 2D @A206 [Chair: Karim Cherifi]

## [02141] Machine Learning for Scientific Discovery, with Examples in Fluid Mechanics

**Format :** Talk at Waseda University

**Author(s) :** Steven Brunton (University of Washington)

**Abstract :** This work describes how machine learning may be used to develop accurate and efficient nonlinear dynamical systems models for complex natural and engineered systems. We explore the sparse identification of nonlinear dynamics (SINDy) algorithm, which identifies a minimal dynamical system model that balances model complexity with accuracy, avoiding overfitting. This approach tends to promote models that are interpretable and generalizable, capturing the essential “physics” of the system.

## [02075] Hamiltonian structure-preserving non-intrusive operator inference for predictive digital twins

**Format :** Talk at Waseda University

**Author(s) :** Anthony Gruber (Sandia National Laboratories)Irina Tezaur (Sandia National Laboratories)Max Gunzburger (University of Texas at Austin)

**Abstract :** To serve as reliable predictive tools, digital twins require dimensionality-reduction techniques that preserve key properties of the underlying equations. This talk presents a novel non-intrusive structure-preserving model reduction technique for canonical and non-canonical Hamiltonian systems based on operator inference. The method reduces to a straightforward linear solve given snapshot data and “gray-box” knowledge of the underlying problem. We demonstrate that, unlike traditional reduction methods, the proposed approach delivers stable, accurate, energy-conserving and robust reduced-order models.

## [01631] Weakly supervised learning for power grid state estimation

**Format :** Talk at Waseda University

**Author(s) :** Jochen Lorenz Cremer (TU Delft)Elvin Isufi (TU Delft)Benjamin Habib (TU Delft)

**Abstract :** In this talk, I present a novel approach for Distribution System State Estimation (DSSE) called the Deep Statistical Solver for Distribution System State Estimation (DSS<sup>2</sup>). This approach, based on graph neural networks (GNNs) and weakly-supervised learning, addresses the challenges of lack of observability and high density in the

part\_2

distribution system. DSS<sup>2</sup> uses hypergraphs to represent the heterogeneous components of the distribution system and updates their latent representations via a node-centric message-passing scheme. Our approach allows for the training of DSS<sup>2</sup> using noisy and corrupted measurements, alleviating the need for ideal labelled data. The results of our experiments on various sizes of power networks showed DSS2 outperforms the conventional Weighted Least Squares algorithm in terms of accuracy, convergence, and computational time and is more robust to noisy, erroneous, and missing measurements. Our approach demonstrates the potential of weakly-supervised learning in DSSE and the ability to respect the physical constraints of the distribution system while learning from noisy measurements.

## [03438] Data-driven Balancing for Acoustical Systems

**Format :** Talk at Waseda University

**Author(s) :** Art J.R. Pelling (TU Berlin)Ennes Sarradj (TU Berlin)

**Abstract :** Constructively modelling acoustical systems is difficult due to unknown material and domain properties and complexity of dynamics. Although measurement data is abundantly available, reduced order modelling is not well-established in the field.

We showcase recent system identification methods from the mathematical community and analyze their aptitude and performance in real applications that involve high-dimensional measurement data. Amongst others, we consider head-related transfer functions that are used for auralization in virtual reality applications.

01099 (3/3) : 2E @A206 [Chair: Ion Victor Gosea]

## [04485] Constrained Optimal Sensing for Nuclear Digital Twins

**Format :** Talk at Waseda University

**Author(s) :** Krithika Manohar (University of Washington)

**Abstract :** We develop a constrained optimization for sensor placement in nuclear digital twins where sensing capability may be severely constrained or limited. These constraints may arise in certain areas of a reactor due to hostile operating conditions, accessibility issues, and physical limitations on sensing capability. Our data-driven method optimizes sensor placement with constraints for full flow field reconstruction, leveraging reduced order models of flow physics. We demonstrate the technique is near optimal using empirical and theoretical validation and provide uncertainty analyses for noisy sensor measurements. The method is demonstrated on a nuclear fuel rod prototype which is heated to mimic the neutronics effect of nuclear fuel within the Transient Reactor Test facility (TREAT) at Idaho National Laboratory.

## [03365] Exploring security challenges in enhancing Digital Twins capabilities with ChatGPT

**Format :** Talk at Waseda University

**Author(s) :** Xingheng Liu (NTNU)Shen Yin (NTNU)Jie Liu (NTNU)Jørn Vatn (NTNU)Asmae Bni (NTNU)

**Abstract :** Digital twins offer valuable insights for monitoring and managing physical systems. With the upsurge of ChatGPT, integrating it with digital twins during the design or operation phase could unlock new capabilities. However, this integration may introduce new security challenges and vulnerabilities. In this talk, we will briefly discuss the potential of enhancing digital twins with ChatGPT and the associated security concerns, emphasizing the importance of addressing these issues to ensure robust, secure DTs.

## [04925] Reduced order modelling for large-scale CFD

**Format :** Talk at Waseda University

**Author(s) :** Zoltán Horváth (Széchenyi István University)Mátyás Yves Constans (Széchenyi István University)

**Abstract :** The RedSim in-house reduced-order modeling (ROM) software for the 3D compressible Euler and Navier-Stokes equations is introduced. RedSim's core consists of a finite volume code running on GPUs and the proper orthogonal decomposition-based ROM-module. The application of RedSim to digital twinning for urban air pollution (in HiDALGO2 EuroHPC Centre of Excellence) and an acoustics problem in the automotive industry are presented. Numerical experiments raise mathematical challenges, which will be presented and some of them solved.

## [04687] Comparison of physics-based and data-driven surrogate models of a gas-bearings supported rotor

**Format :** Online Talk on Zoom

**Author(s) :** Dimitri Goutaudier (EPFL)Jürg Schiffmann (EPFL)Fabio Nobile (EPFL)

**Abstract :** Gas bearings use pressurized gas as a lubricant to support and guide rotating machinery. These bearings have several advantages over traditional lubricated bearings but they are more complex to operate and exhibit nonlinear behaviors. In this contribution, we present physics-based and data-driven frameworks to compute the dynamics of a gas-bearings supported rotor operating at very high rotation speeds. We compare the numerical performances of the two approaches, and we propose research directions to improve the models.

## [01107] Efficient methods for Isogeometric Analysis

**Session Time & Room :**

01107 (1/2) : 2D (Aug.22, 15:30-17:10) @G301

01107 (2/2) : 2E (Aug.22, 17:40-19:20) @G301

**Type :** Proposal of Minisymposium

**Abstract :** Isogeometric Analysis is a relatively novel technique used to solve PDEs. The same functions that are used to describe the computational domain (typically B-Splines or NURBs) are used also to approximate the solution of the considered PDE. This approach brings several advantages with respect to the classical finite element method, but it also leads to new challenges, in particular from the computational point of view. This minisymposium aims at gathering researchers that contribute to the improvement of the efficiency for isogeometric methods.

**Organizer(s) :** Mattia Tani, John Evans, Angelos Mantzaflaris, Stefan Takacs

**Classification :** 65N30, 65Y20, 65N38

**Minisymposium Program :**

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01107 (1/2) : 2D @G301

## [04261] Matrix free weighted quadrature IgA applied to heat transfer problems

**Author(s) :** Joaquin Eduardo Cornejo Fuentes (INSA Lyon)Thomas Elguedj (Lamcos)Arnaud Duval (Lamcos)David Dureisseix (Lamcos)

**Abstract :** IsoGeometric Analysis was introduced as an extension of Finite Element Method to represent the geometry and the solution field. However, the algorithms commonly used in FEM represented a major challenge from a computational point of view in IgA. This communication focuses on novel techniques applied to heat transfer problems which take advantage of the tensor structure of the shape functions, improve computation time of matrix-vector products and enhance the convergence rate of the iterative solver.

## [04410] Solving boundary value problems via the Nystrom method using spline Gauss rules

**Author(s) :** Michael Barton Ali Hashemian (BCAM)Hanna Sliusarenko (BCAM)Sara Remogna (University of Torino)Domingo Barrera (University of Granada)

**Abstract :** We propose to use spline Gauss quadrature rules for solving boundary value problems~(BVPs) using the Nystrom method. When solving BVPs, one converts the corresponding partial differential equation inside a domain into the

Fredholm integral equation of the second kind on the boundary in the sense of boundary integral equation (BIE). The Fredholm integral equation is then solved using the Nystrom method, which involves the use of a particular quadrature rule, thus, converting the BIE problem to a linear system. We demonstrate this concept on the 2D Laplace problem over domains with smooth boundary as well as domains containing corners. We validate our approach on benchmark examples and the results indicate that, for a fixed number of quadrature points (i.e., the

same computational effort), the spline Gauss quadratures return an approximation that is by one to two orders of magnitude more accurate compared to the solution obtained by traditional polynomial Gauss counterparts.

## [04643] Fast computation of electromagnetic wave propagation with spline differential forms

**Author(s)** : Bernard Kapidani (Ecole Polytechnique Fédérale Lausanne)Rafael Vazquez (Ecole Polytechnique Fédérale Lausanne)

**Abstract** : We present a new structure-preserving numerical method for hyperbolic problems which does not rely on the geometric realisation of any dual mesh. We use B-spline based de Rham complexes to construct two exact sequences of discrete differential forms and apply them to solving Maxwell's equations. The method exhibits high order convergence and energy conservation, with computational effort much lower than standard Galerkin. We will also present preliminary results towards extension to multi-patch geometries.

## [04698] Isogeometric Coupling Methods for H(curl) Problems

**Author(s)** : Melina Merkel (Technische Universität Darmstadt)Sebastian Schöps (Technische Universität Darmstadt)

**Abstract** : In this work, we present a method for the efficient simulation of electric motors using isogeometric analysis. As these machines include moving parts, conformity of the patches cannot be guaranteed for all rotation angles without modification of the geometry. We therefore use domain decomposition methods, e.g., mortaring or Nitsche-type coupling, for the coupling of stator and rotor. These methods can also be applied to all patches to facilitate patch-parallel computations.

01107 (2/2) : 2E @G301

## [05111] Efficient reduced order models for unfitted spline discretizations

**Author(s)** : Margarita Chasapi (EPFL)Pablo Antolin (EPFL)Annalisa Buffa (EPFL)

**Abstract** : This talk presents a methodology for efficient reduced order modelling of PDEs on unfitted spline discretizations. We are interested in problems formulated on parameterized unfitted geometries and aim to construct efficient reduced basisapproximations. The presented methodology is based on extension of solution snapshots on the background mesh and localization strategies to confine the number of reduced basis functions. Numerical experiments on trimmed spline discretizations show the accuracy and efficiency of the method.

## [05187] Singularity extraction and efficient numerical integration for isogeometric BEM

**Author(s)** : Tadej Kanduc (University of Ljubljana)

**Abstract** : Quadrature rules to evaluate governing (weakly singular) integrals that appear in boundary integral equations for 3D potential problems are presented. The rules are described by two main features: a higher order isoparametric singularity extraction technique and a spline-based quasi-interpolation technique. Uniform distribution of quadrature nodes is preferable to improve the implementation efficiency. The integration scheme has high order converge rates and since it is tailored for spline integrands, it perfectly fits in the isogeometric framework.

## [05212] Low-rank Tensor Train Methods for IGA with Multiple Patches

**Author(s)** : Alexandra Bünger (University of British Columbia)Martin Stoll (Technical University of Chemnitz)Tom Christian Riemer (Technical University of Chemnitz)

**Abstract** : In IGA, the equation systems for, e.g., optimization problems may quickly become very costly to assemble and solve. We developed a method exploit the underlying tensor structure with low-rank tensor train approximations. This low-rank formulation can be efficiently used in a block-structured iterative solver to solve challenging PDE problems in a compact format.

We recently extended this for multi-patch domains and show how the resulting systems can be treated effectively in the tensor train framework.

## [05302] An efficient solver for space-time isogeometric Galerkin methods for parabolic problems

**Author(s)** : Gabriele Loli (Università di Pavia )Monica Montardini (Università di Pavia )Giancarlo Sangalli (Università di Pavia )Mattia Tani (University of Pavia)

**Abstract** : We present an efficient solver for a Galerkin space-time isogeometric discretization of the heat equation. In particular, we propose a preconditioner that is the sum of Kronecker products of matrices and that can be efficiently applied thanks to an extension of the classical Fast Diagonalization method.

The preconditioner is robust w.r.t. the polynomial degree of the spline space and the time required for the application is almost proportional to the number of degrees-of-freedom.

## [01111] Mathematical and numerical analysis on blow-up phenomena

**Session Time & Room :**

01111 (1/2) : 4C (Aug.24, 13:20-15:00) @G501

01111 (2/2) : 4D (Aug.24, 15:30-17:10) @G501

**Type** : Proposal of Minisymposium

**Abstract** : Blow-up phenomena appear in various science fields. They are described by partial differential equations. It is difficult to construct a general theory for the blow-up phenomena of partial differential equations. Therefore, we need to approach them from both mathematical and numerical aspects. In this mini-symposium, we discuss blow-up time and blow-up profile from the perspectives of mathematical and numerical analysis. The purpose of this minisymposium is to bring together researchers from both mathematical and numerical analysis to discuss recent advances on blow-up phenomena.

**Organizer(s)** : Takiko Sasaki

**Classification** : 35B44, 35A35, 35K05, 35L71

**Minisymposium Program :**

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01111 (1/2) : 4C @G501 [Chair: Takiko Sasaki]

## [01625] On the convergence order of the numerical blow-up time

**Author(s)** : Chien-Hong Cho (National Sun Yat-sen University)

**Abstract** : It is quite often that the solutions of initial-value problems become unbounded in a finite time. Such a phenomenon is called blow-up and the finite time is called the blow-up time. In this talk, we put our attention on the computation of an approximate blow-up time and its convergence order.

## [01957] The blow-up curve for systems of semilinear wave equations

**Author(s)** : Takiko Sasaki (Department of Mathematical Engineering, Faculty of Engineering, Musashino University and Mathematical Institute, Tohoku University)

**Abstract** : In this talk, we consider a blow-up curve for systems of semilinear wave equations with different propagation speeds in one space dimension. The blow-up curve has been studied from the view point of its differentiability and singularity. We show that the blow-up curve has a singular point under suitable initial conditions. We also show some numerical examples of blow-up curves.

## [01774] Lifespan estimates of semilinear wave equations of derivative type with characteristic weights in one space dimension

**Author(s)** : Shunsuke Kitamura (Tohoku University, Graduate School of Science)

**Abstract** : In this talk, I discuss the initial value problems for semilinear wave equations of derivative type with characteristic weights in one space dimension. Such equations provide basic principles on extending the general theory for nonlinear wave equations to the non-autonomous case. The results are quite different from the results of a series of joint work with Takamura, Wakasa and Morisawa about the nonlinear terms of unknown function itself.

## [01740] On degenerate blow-up profiles for the semilinear heat equation

**Author(s)** : Hatem Zaag (CNRS and Université Sorbonne Paris Nord)

**Abstract** : We consider the semilinear heat equation with a superlinear power nonlinearity in the Sobolev subcritical range. We construct a solution which blows up in finite time only at the origin, with a completely new blow-up profile, which is cross-shaped. Our method is general and extends to the construction of other solutions blowing up only at the origin, with a large variety of blow-up profiles, degenerate or not.

01111 (2/2) : 4D @G501 [Chair: Takiko Sasaki]

## [03241] Collapse Versus Blowup and Global Existence in Generalized Constantin–Lax–Majda Equation with dissipation

**Format** : Online Talk on Zoom

**Author(s)** : Pavel M Lushnikov (University of New Mexico)David M Ambrose (Drexel University)Michael Siegel (Department of Mathematical Sciences and Center for Applied Mathematics and Statistics, New Jersey Institute of Technology,)Denis A Silantyev (Department of Mathematics, University of Colorado, Colorado Springs.)

**Abstract** : We analyze dynamics of singularities and finite time blowup of generalized Constantin-Lax-Majda equation for non-potential effective motion of fluid with competing convection, vorticity stretching and dissipation. Multiple exact solutions are found with blowups. Global existence of solutions is proven for small data in periodic case. The analytical solutions on real line allow finite-time singularity formation for arbitrarily small data illustrating critical difference between real line and periodic cases. Analysis is complemented by accurate numerical simulations.

## [01136] Advances in Variational Models and PDEs for Images

**Session Time & Room** :

01136 (1/3) : 4C (Aug.24, 13:20-15:00) @E819

01136 (2/3) : 4D (Aug.24, 15:30-17:10) @E819

01136 (3/3) : 4E (Aug.24, 17:40-19:20) @E819

**Type** : Proposal of Minisymposium

**Abstract** : Variational models and partial differential equations have been used to model various aspects of images, and this has led to many effective approaches to solve diverse image processing problems, such as image denoising, segmentation, reconstruction. This minisymposium will provide a venue for the latest advances in analysis and algorithm design for variational models and PDEs, and we will showcase state-of-the-art applications in image processing.

**Organizer(s)** : Gunay Dogan, Ronald Lok Min Lui

**Classification** : 68U10, 65D18, 62H35, 94A08, 68T45

**Minisymposium Program** :

01136 (1/3) : 4C @E819 [Chair: Gunay Dogan]

## [03732] Algorithms for Variational Segmentation of Regions and Boundaries

**Format** : Talk at Waseda University

**Author(s)** : Gunay Dogan (National Institute of Standards and Technology)

**Abstract** : We propose several algorithms for variational segmentation of regions and boundaries in images. The algorithms come in Lagrangian and Eulerian flavors, and optimize variational models incorporating boundaries

and region statistics, as well as various geometric regularizers. We demonstrate the advantages of each algorithm on several examples. Our algorithms are available in the open-source Python package scikit-shape.

## [04275] Individual Tooth Segmentation in Human Teeth Images Using Pseudo Edge-Region Obtained by Deep Neural Networks

**Format :** Talk at Waseda University

**Author(s) :** Chang-Ock Lee (KAIST)Seongeun Kim (KAIST)

**Abstract :** In human teeth images taken outside the oral cavity with a general optical camera, it is difficult to segment individual tooth due to common obstacles such as weak edges, intensity inhomogeneities and strong light reflections. In this talk, we propose a method for segmenting individual tooth in human teeth images. The key to this method is to obtain pseudo edge-region using deep neural networks.

## [05117] Joint solution of multi-task problems in imaging

**Format :** Talk at Waseda University

**Author(s) :** Doga Gursoy (Argonne National Laboratory)

**Abstract :** Imaging in challenging conditions, such as with limited and uncertain data, typically involves solving multiple tasks, including image denoising, registration, segmentation, and various other reconstruction tasks. While the traditional approach has been to address these problems one at a time, solving them jointly with minimal manual hyperparameter setting can provide significant benefits in terms of image quality and acquisition time. In this presentation, I will explore the use of distributed optimization techniques to tackle these challenges and offer examples from my experience in the field of x-ray imaging.

## [01799] Counting Objects by Diffused Index: geometry-free and training-free approach

**Format :** Talk at Waseda University

**Author(s) :** Maryam Yashtini (Georgetown University)

**Abstract :** Counting objects is a fundamental but challenging problem. In this talk, I propose diffusion-based, geometry-free, and learning-free methodologies to count the number of objects in images. The main idea is to represent each object by a unique index value regardless of its intensity or size, and to simply count the number of index values. First, I place different vectors, referred to as seed vectors, uniformly throughout the mask image. The mask image has boundary information of the objects to be counted. Secondly, the seeds are diffused using an edge-weighted harmonic variational optimization model within each object. I propose an efficient algorithm based on an operator splitting approach and alternating direction minimization method, and theoretical analysis of this algorithm is given. An optimal solution of the model is obtained when the distributed seeds are completely diffused such that there is a unique intensity within each object, which I refer to as an index. For computational efficiency, I stop the diffusion process before a full convergence, and propose to cluster these diffused index values. I refer to this approach as Counting Objects by Diffused Index (CODI). I explore scalar and multi-dimensional seed vectors. For Scalar seeds, I use Gaussian fitting in histogram to count, while for vector seeds, I exploit a high-dimensional clustering method for the final step of counting via clustering. The proposed method is flexible even if the boundary of the object is not clear nor fully enclosed. I present counting results in various applications such as biological cells, agriculture, concert crowd, and transportation. Some comparisons with existing methods are presented.

01136 (2/3) : 4D @E819 [Chair: Gunay Dogan]

## [04373] A deep quasiconformal approach for topological preserving image segmentation

**Format :** Online Talk on Zoom

**Author(s) :** Ronald Lok Ming LUI (The Chinese University of Hong Kong)

**Abstract :** In this talk, we address the problem of topology-preserving image segmentation based on quasiconformal (QC) theories. We introduce a variational model to obtain an optimal QC map that deforms a template mask to the segmentation mask while preserving the topology of the template mask. The bijectivity of the mapping is controlled by the Beltrami coefficient, which measures the QC distortion. We demonstrate that the proposed QC segmentation model can be effectively incorporated into a deep neural network architecture. The resulting deep QC segmentation network takes an image and a template mask with a prescribed topological prior as inputs and outputs the optimal QC map. The QC map is further used to deform the template mask to obtain the segmentation result. Experimental results show that the proposed approach outperforms existing state-of-the-art

part\_2

methods, making it a promising approach for topological preserving image segmentation. This work is supported by HKRGC GRF (Project IDs: 14306721,14307622).

## [02523] Geodesic Models with Curvature Penalization for Image Analysis

**Format :** Talk at Waseda University

**Author(s) :** Da CHEN (Shandong Artificial Intelligence Institute)

**Abstract :** Geodesic models establish the connection between the minimization of a weighted curve length and the viscosity solutions to the HJB PDEs. In contrast to globally minimizing a simplified first-order energy, as done by the classical geodesic models, we have recently extended the geodesic models to cover different curvature regularization terms, in conjunction with convexity shape prior and curvature prior constraint. We also show their applications in tubular structure tracking and image segmentation.

## [02808] Texture edge detection via Patch consensus

**Format :** Talk at Waseda University

**Author(s) :** Guangyu Cui (Georgia Institute of Technology) Sung Ha Kang (Georgia Institute of Technology)

**Abstract :** While well-known segmentation method are often based on homogeneity of regions, we focus on finding boundaries between different textured regions. We propose a training-free method to detect the boundary of texture by considering consensus of patch responses away from the boundary. We derive the necessary condition for textures to be distinguished, and analyze the size of the patch with respect to the scale of textures. Various experiments are presented to validate our model.

## [04153] Density-equalizing map with applications

**Format :** Talk at Waseda University

**Author(s) :** Gary Choi (The Chinese University of Hong Kong)

**Abstract :** We present surface and volumetric mapping methods based on a natural principle of density diffusion. Specifically, we start with a prescribed density distribution in a surface or volumetric domain, and then create shape deformations with different regions enlarged or shrunk based on the density gradient. By changing the density distribution, we can achieve different mappings including area-preserving parameterizations. Applications of the methods to medical shape analysis, data visualization, remeshing and shape morphing will be presented.

01136 (3/3) : 4E @E819 [Chair: Gunay Dogan]

## [01712] Application of weighted TV flow to material science problems

**Format :** Online Talk on Zoom

**Author(s) :** Prashant Athavale (Clarkson University) Emmanuel Atindama (Clarkson University) Peter Lef (Clarkson University) Gunay Dogan (National Institute of Standards and Technology)

**Abstract :** Several variational and partial differential equation (PDE)-based image processing methods can restore noisy crystallographic orientation data.

We discuss restoration approaches, such as the classical total variation-based methods to diffusion PDEs.

However, such methods are parameter-dependent, making them challenging in practice.

Our work discusses an algorithm to restore noisy orientation data and circumvent the parameter selection problem by using weighted total variation flow, a nonlinear diffusion applied to the noisy orientation map.

## [04202] Rank-One Prior: Real-Time Scene Recovery

**Format :** Talk at Waseda University

**Author(s) :** Tieyong Zeng (The Chinese University of Hong Kong)

**Abstract :** Scene recovery is a fundamental imaging task with several practical applications, including video surveillance and autonomous vehicles, etc. In this talk, we provide a new real-time scene recovery framework to restore degraded images under different weather/imaging conditions, such as underwater, sand dust and haze. A degraded image can actually be seen as a superimposition of a clear image with the same color imaging environment (underwater, sand or haze, etc.). Mathematically, we can introduce a rank-one matrix to characterize this phenomenon, i.e., rank-one prior (ROP). Using the prior, a direct method with the complexity is derived for real-time recovery. For general cases, we develop ROP to further improve the recovery performance. Comprehensive experiments of the scene recovery illustrate that our method outperforms competitively several state-of-the-art imaging methods.

## [02233] Multispectral Image Restoration by Structured Eigendecomposition

**Format :** Talk at Waseda University

**Author(s) :** Zhantao MA (The University of Hong Kong) Michael Kwok-Po NG (The University of Hong Kong)

**Abstract :** We propose and study the opponent transformation for multispectral images. We generalize the well-known opponent transformation for color images and use it to bring the generalized opponent transformation total variation (GOTTV) multispectral image restoration model. By inheriting the crucial properties of the opponent transformation, the minimization formula of the GOTTV can be simplified and solved by the ADMM. Numerical examples are presented to demonstrate that the performance of the new GOTTV is well.

## [01138] Advances in embedded and Eulerian methods for fluid-structure interaction

**Session Time & Room :** 4C (Aug.24, 13:20-15:00) @E820

**Type :** Proposal of Minisymposium

**Abstract :** This mini-symposium brings together young researchers and experts working on numerical modeling of fluid-structure interaction problems. To avoid the remeshing step involved in ALE method, other approaches based on non-body fitted grids have become more and more attractive. One is the embedded approach where a Lagrangian structure solver interacts with an Eulerian fluid solver to enforce appropriate conditions on the immersed interface. Another one is the fully Eulerian approach where both the fluid and the elastic structure are discretized on the same grid. This mini-symposium welcomes contributions to embedded and fully Eulerian numerical modelling for both compressible and incompressible FSI.

**Organizer(s) :** Michel Bergmann, Thomas Milcent

**Classification :** 76-XX, 74-XX, 65-XX, 68-XX, fluid structure interaction, embedded methods, fully Eulerian models

**Minisymposium Program :**

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01138 (1/1) : 4C @E820 [Chair: Bergmann Michel]

### [05651] A fully Eulerian FSI framework: introduction

**Format :** Talk at Waseda University

**Author(s) :** Thomas Milcent (I2M Bordeaux) Michel Bergmann (Inria - centre de l'université de Bordeaux)

**Abstract :** In the fully Eulerian framework, both the fluid and the solid are described by an Eulerian approach. The fluid-structure problem is recast as a complex flow: the fluid equations with an elastic source term is coupled with a transport equation on the Eulerian interface and deformation. In this presentation we will present this approach in the case where the elastic media (bulk or/and membrane) is immersed in an incompressible or compressible flow.

### [05652] A fully Eulerian FSI framework: numerical approach and applications

**Format :** Talk at Waseda University

**Author(s) :** Michel Bergmann (Inria - centre de l'université de Bordeaux) Thomas Milcent (I2M Bordeaux) Antoine Fondaneche (NUREA)

**Abstract :** A quadtree-based fully Eulerian finite volume approach for the simulation of fluid-structure interaction problems is presented. The discretization stencils are limited to the first layer of neighbors thus enhancing the efficiency of the parallel computations while limiting the numerical order of the finite volume discretizations that can be reached. To illustrate the versatility of the numerical model presented, a biomedical application, the axisymmetric simulation of a blood flow in a cardiac pump, is presented.

## [02558] Embedded Methods for Floating Offshore Structures

**Format :** Talk at Waseda University

**Author(s) :** Jan Modderman (Delft University of Technology)Oriol Colomés (Delft University of Technology)

**Abstract :** In this talk we will present a single-phase FE approach for free surface flows, where only the wave-structure interaction is accounted for, in combination with an unfitted floating structure with arbitrary geometry. In this work we propose a monolithic coupling with block preconditioning, ensuring robustness and efficiency of the solution. We will demonstrate the capabilities of the proposed framework with a series of tests for wave-structure interaction problems, assessing accuracy and conservation properties.

## [03927] FULLY EULERIAN MODELS FOR FLUID-STRUCTURE INTERACTION: APPLICATION TO CAPSULES

**Format :** Talk at Waseda University

**Author(s) :** Mirco Ciallella (ENSA - I2M)Thomas Milcent (ENSA - I2M)

**Abstract :** Capsules have an important potential in the fields of biotechnologies but many scientific aspects, related to their modeling and simulation, are still challenging. In this context, eulerian models for fluid-structure interaction are a very promising tool to understand their behavior when interacting with complex geometries. In this talk, we will present a novel numerical tool to analyze complex applications of deformable capsules by introducing a solid bulk within the membrane.

## [01140] Modelling and simulation of electro-chemo-mechanical processes in batteries and fuel cells

**Session Time & Room :**

01140 (1/3) : 5B (Aug.25, 10:40-12:20) @G404

01140 (2/3) : 5C (Aug.25, 13:20-15:00) @G404

01140 (3/3) : 5D (Aug.25, 15:30-17:10) @G404

**Type :** Proposal of Minisymposium

**Abstract :** The mini-symposium addresses various aspects of modelling and simulation of electro-chemo-mechanical processes in batteries and fuel cells. It is aimed at scientists from academia and industry and focuses on the physical and mathematical fundamentals of the processes rather than the system level. Aspects such as model derivation at the microscopic level and its upscaling, model validation and model reduction are the focus of this mini-symposium. It covers contributions on lithium and sodium ion and redox flow batteries, solid oxide and polymer electrolyte fuel cells, among others.

**Organizer(s) :** Thomas Carraro, Manuel Landstorfer, Yosuke Komatsu

**Classification :** 35-04, 65-04, Modelling electrochemical processes

**Minisymposium Program :**

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01140 (1/3) : 5B @G404 [Chair: Thomas Carraro]

## [01934] Li-Ion battery kinetics model validation of NMC 111 and Graphite

**Format :** Talk at Waseda University

**Author(s) :** Robert Morasch (Technical University of Munich)Bharatkumar Suthar (Indian Institute of Technology Bombay)Hubert Gasteiger (Technical University of Munich)

**Abstract :** Understanding Li-Ion battery fundamentals is an important aspect when modelling Li-Ion batteries. The Doyle-Fuller-Newman model is often used as mathematical basis for such models, but rarely validated. Here we present an in-depth analysis of the kinetic behavior of NMC 111 and graphite using Electrochemical Impedance Spectroscopy. Measurements on thin electrodes allow an easy distinction of the kinetic resistance for either electrode without the influence of transport resistances.

## [04354] Fluid-electrochemical-stress-coupled Simulation Method for SOFC Degradation Prediction

**Format :** Talk at Waseda University

**Author(s) :** Mayu Muramatsu (Keio University)Masami Sato (Tohoku University)Reika Nomura (Tohoku University)Kenjiro Terada (Tohoku University)Yashiro Keiji (Tohoku University)Tatsuya Kawada (Tohoku University)Harumi Yokokawa (The University of Tokyo)

**Abstract :** To predict the mechanical degradation of solid oxide fuel cells (SOFCs) during operation, we have developed an analysis system for their electro-chemo-mechanical phenomena by incorporating general-purpose finite element analysis software. This simulation system also takes into account the effects of gas and heat distributions, also calculated by commercial software.

## [02306] Modeling and State Estimation of Lithium-Ion Batteries under Long-Term Degradation Conditions in Aerospace Application

**Format :** Talk at Waseda University

**Author(s) :** Linda Juliane Bolay (German Aerospace Center (DLR))Tobias Schmitt (German Aerospace Center (DLR))Simon Hein (German Aerospace Center (DLR))Omar Mendoza-Hernandez (Japan Aerospace Exploration Agency (JAXA))Eiji Hosono (National Institute of Advanced Industrial Science and Technology (AIST))Daisuke Asakura (, National Institute of Advanced Industrial Science and Technology (AIST))Koichi Kinoshita (, National Institute of Advanced Industrial Science and Technology (AIST))Hirofumi Matsuda (, National Institute of Advanced Industrial Science and Technology (AIST))Minoru Umeda (Nagaoka University of Technology)Yoshitsugu Sone (Japan Aerospace Exploration Agency (JAXA))Arnulf Latz (German Aerospace Center (DLR))Birger Horstmann (German Aerospace Center (DLR))

**Abstract :** The performance and durability of Li-ion batteries is impacted by various degradation mechanisms such as SEI growth. Here, we address the modeling and simulation of the batteries of the Japanese satellite REIMEI. We simulate SEI growth in a P2D and microstructure-resolved framework. The simulations are validated with in-flight data from JAXA. Furthermore, a multi-time-scale filter algorithm is applied to estimate the inner states of the battery by making use of the battery in-flight data.

## [02922] Simulation of Chemo-Mechanically Coupled Battery Active Particles with Mechanical Constraints

**Format :** Talk at Waseda University

**Author(s) :** Raphael Schoof (Karlsruhe Institute of Technology)Giuseppe Fabian Castelli (Karlsruhe Institute of Technology)Willy Dörfler (Karlsruhe Institute of Technology)

**Abstract :** During charging and discharging of lithium-ion batteries, large mechanical stresses can occur due to phase-separation or limited swelling area. A chemo-mechanically coupled model for cycling battery active particles with mechanical constraints is used to investigate the stress development within representative active particles. The combination of the primal-dual active set algorithm, interpreted as semismooth Newton method, and a spatial and temporal adaptive algorithm allows the efficient two- and three-dimensional numerical simulation and computationally intensive parameter regimes.

01140 (2/3) : 5C @G404 [Chair: Thomas Carraro]

## [04773] Electro-chemical based modelling of battery cells for automotive applications.

**Format :** Online Talk on Zoom

**Author(s) :** Edwin Knobbe (BMW AG)

**Abstract :** This contribution presents challenges with respect to modelling and (numerical) simulations of the interaction of mechanics and electro-chemistry for applications in battery cell development. Some of the challenges will be explained by examples relevant for automotive applications. For instance: solid mechanics to model the swelling behavior of battery cells during cycling, fluid mechanics with detailed chemistry during a thermal event and modelling electro-chemical phenomena at the interface between an electrode and a solid electrolyte.

## [02597] Analytical solution to a multilayer particle model for Li-ion cells under generic high current profiles

**Format :** Online Talk on Zoom

**Author(s) :** Javid Piruzjam (Mercedes-Benz AG)Lukas Rubacek (Mercedes-Benz AG)Thomas Carraro (Helmut Schmidt University / UniBw Hamburg)

**Abstract :** Reduced order Li-ion battery models are widely used in applications such as state of charge estimation by electric vehicles' battery management systems, or cell characterization. Among those models, Single Particle Model is a computationally inexpensive physics-based solution. However, neglecting the effect of the electrolyte dynamics on the cell performance, SPM can lead to large errors especially at high current applications. In this work, we propose an analytical solution to a single particle model including electrolyte dynamics (SPMe) which is applicable for a wide range of currents. The boundary conditions and source terms in all differential equations are time-varying, and a spherical multilayer diffusion scenario is also considered which allows modelling particles coating and degradation effect.

## [03013] Exploring non-isothermal effects in all-vanadium redox flow batteries through advanced numerical models

**Format :** Online Talk on Zoom

**Author(s) :** Marcos Vera (Universidad Carlos III de Madrid)Vanesa Muñoz-Perales (Universidad Carlos III de Madrid)Santiago E. Ibáñez (Repsol)Enrique García-Quismondo (IMDEA Energy)Sabrina Berling (IMDEA Energy)Jesús Palma (IMDEA Energy)

**Abstract :** Redox flow batteries are a promising electrochemical technology for large-scale stationary energy storage that still requires further development to increase its profitability and energy market penetration. Continuous macroscopic models enable the optimization of new architectures and operational strategies without extensive fabrication and experimental procedures. This work presents a non-isothermal two-dimensional steady-state model of a unit-cell all-vanadium redox flow battery. The model integrates state-of-the-art descriptions of the fundamental physical phenomena along with new features, such as local mass transfer coefficients for the active species, precise sulfuric acid dissociation kinetics, and experimentally determined electrochemical parameters and electrolyte properties. The model is validated at different states of charge, flow rates, and operating temperatures using polarization, conductivity, and open circuit voltage measurements. Then, the contribution of operating conditions to battery performance is studied by analyzing its separate effect on the various phenomena that affect cell performance, such as local pore mass transfer limitations, parasitic hydrogen evolution reactions, crossover, and self-discharge fluxes. After model calibration, a parametric study is carried out to explore the role of the operating temperature, deconvoluting the different contributions to cell heating and providing practical guidance about the thermal effects induced by operating conditions. The results reveal that i) increasing the cell temperature enhances species mass transfer but negatively affects activation losses, ii) the cell suffers higher overheating during charge than during discharge, and iii) cell heating increases proportionally with cell length. Lastly, we propose using asymmetric electrolyte temperatures as a performance improvement strategy for electrochemical storage systems hybridized with thermal energy storage. The resulting model is a reliable tool that can be used to assess the relevance of the coupled phenomena that take place simultaneously within the reaction cell. This vital information is critical to optimize cell components, reactor design and selecting optimal operating conditions.

## [03277] A Model Framework for Lithium Ion Intercalation Cells

**Format :** Talk at Waseda University

**Author(s) :** Manuel Landstorfer (Weierstrass Institute for Applied Analysis and Stochastics (WIAS))Alireza Selahi (Weierstrass Institute for Applied Analysis and Stochastics (WIAS))

**Abstract :** We present a model framework for Lithium-ion batteries based on non-equilibrium thermodynamics. It emphasizes thermodynamic consistency, especially for reaction rates and concentration-dependent diffusion coefficients. A coupled two-scale PDE system is derived using periodic homogenization. Numerical simulations are finally shown, predicting the cell voltage during cycling at different C-Rates. We compare single- and many-particle electrode models and discuss the impact of material functions, diffusion coefficients, and reaction rate models based on numerical simulations.

## [02810] Asymptotic reduction of a model for mechanical stresses in cylindrical batteries

**Format :** Talk at Waseda University

**Author(s) :** Jon Chapman (University of Oxford)Robert Timms (University of Oxford)Steven Psaltis (Queensland University of Technology)Colin Please (University of Oxford)

**Abstract :** Macroscopic mechanical stresses in lithium-ion batteries are known to significantly affect the long-term degradation mechanisms. These stresses are created by expansion and contraction of the different parts of the structure, due both to thermal variations and lithiation state. Predicting the resulting stresses using numerical techniques is made difficult due to the small-scale geometry of current collectors, separator and regions of active material.

Here we use the methods of boundary layer analysis and homogenisation, exploiting the small-scale periodic structure of a spirally-wound cylindrical battery, to derive a reduced-order model to determine approximations to the resulting stresses.

## [05025] Microstructural resolved simulations of NVP-C electrodes for Sodium-ion batteries

**Format :** Talk at Waseda University

**Author(s) :** Paul Maidl (German Aerospace Center)Simon Hein (German Aerospace Center)Timo Danner (German Aerospace Center)Matthias Neumann (University Ulm)Marcel Häringer (Karlsruhe Institute of Technology )Luca Schneider (Karlsruhe Institute of Technology )Werner Bauer (Karlsruhe Institute of Technology )Ingo Manke (Helmholtz-Zentrum Berlin)Volker Schmidt (University Ulm)Joachim R. Binder (Karlsruhe Institute of Technology )Arnulf Latz (German Aerospace Center)

**Abstract :** Sodium-ion batteries are a promising candidate for sustainable future energy storage technologies. Although they have some similarities with Lithium ion batteries, today's modelling and simulation techniques for Sodium-ion batteries is lacking behind their Lithium counterpart. One interesting material for both anode and cathode is NVP-C ( $Na_3V_2(PO_4)_3$  with added carbon). In our contribution we show simulation approaches for virtual material characterization of its complex three-dimensional microstructure and its influence on cell performance.

## [04382] Modeling Solid Oxide Fuel Cells based on Electrode Microstructure Information

**Format :** Talk at Waseda University

**Author(s) :** Masashi Kishimoto (Kyoto University)Hiroshi Iwai (Kyoto University)

**Abstract :** Understanding the effect of the porous microstructure of SOFC electrodes on the electrochemical performance is essential in predicting their macroscopic performance and thereby optimizing electrode microstructure. We present several numerical simulation models of SOFCs with quantitative information of the electrodes obtained by 3D imaging technique based on focused ion beam scanning electron microscope (FIB-SEM). Typical results of microscopic distribution within the electrodes and macroscopic performance, such as overpotential and impedance characteristics, are overviewed.

## [05164] Improving Lithium-ion Battery Models for Porous Secondary Particles: A Comparison of Homogenized and Microscopic 3D Models

**Format :** Talk at Waseda University

**Author(s) :** Javid Piruzjam (Mercedes-Benz AG)Phillip Gräfensteiner (Ulm University)Matthias Neumann (Ulm University)Lukas Rubacek (Mercedes-Benz AG)Volker Schmidt (Ulm University)Thomas Carraro (Helmut Schmidt University / UniBw Hamburg)

**Abstract :** We present a study on a homogenized model for porous secondary particles of lithium-ion batteries in comparison with microscopic 3D models. The 3D microstructures are based on FIB-SEM tomography, which provides high-resolution images of the secondary particles. Homogenized electrode-level models are widely used in battery applications due to their computational efficiency, e.g., in the electric vehicle industry. However, the accuracy of these models can be improved if the transport processes within the porous particles are considered, especially when complex microstructures are involved. Our investigation aims to improve the quantitative prediction of multiscale models. To perform a comprehensive study, we use digital twins to obtain adequate stochastic representations of the microstructure.

# [01145] High dimensional recent computational approaches in finance and control

## **Session Time & Room :**

01145 (1/2) : 5B (Aug.25, 10:40-12:20) @D505

01145 (2/2) : 5C (Aug.25, 13:20-15:00) @D505

## **Type :** Proposal of Minisymposium

**Abstract :** Most high-dimensional problem in quantitative finance face computational difficulties. However, recent advances in training of neural networks provide an excellent opportunity to reconsider these models. Indeed, the influential papers of E, Han and Jentzen combine these optimization techniques with Monte-Carlo type regression for the off-line construction of optimal feedback actions. This approach, has proven to be highly effective in numerous closely related studies, reporting impressive numerical results in problems with large number of states.

All proposed speakers have been contacted and agreed to participate in the session should it be approved. This list of speakers is diverse in many ways, including both senior and junior members of the community and also it represents several different scientific approaches.

**Organizer(s) :** A. Max Reppen, H. Mete Soner  
**Sponsor :** This session is sponsored by the SIAM Activity Group on Financial Mathematics and Engineering.

**Classification :** 91G60, 49N35, 65C05

## **Minisymposium Program :**

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01145 (1/2) : 5B @D505 [Chair: H. Mete Soner]

# [03950] Learning to Simulate Tail-Risk Scenarios

## **Format :** Talk at Waseda University

**Author(s) :** Rama Cont (University of Oxford)Mihai Cucuringu (University of Oxford)Renyuan Xu (University of Southern California)Chao Zhang (University of Oxford)

**Abstract :** The estimation of loss distributions for dynamic portfolios requires the simulation of scenarios representing realistic joint dynamics of their components. Scalability to large or heterogeneous portfolios involving multiple asset classes is particularly challenging, as is the accurate representation of tail risk.

We propose a novel data-driven approach for the simulation of realistic multi-asset scenarios with a particular focus on the accurate characterization of tail risk for a given class of static and dynamic portfolios selected by the user. By exploiting the joint elicibility property of Value-at-Risk (VaR) and Expected Shortfall (ES), we design a Generative Adversarial Network (GAN) architecture capable of learning to simulate price scenarios that preserve tail risk features for these benchmark trading strategies, leading to consistent estimators for their VaR and ES.

From a theoretical perspective, we show that different choices of score functions lead to different optimization landscapes and different complexities in GAN training. In addition, we prove that the generator in our GAN architecture enjoys a universal approximation property under the criteria of tail risk measures. In addition, we prove the bi-level optimization formulation between the generator and the discriminator is equivalent to a max-min game, leading to a more effective and practical formulation for training. From an empirical perspective, we demonstrate the accuracy and scalability of our method via extensive simulation experiments using synthetic and market data. Our results show that, in contrast to other data-driven scenario generators, our proposed scenario simulation method correctly captures tail risk for both static and dynamic portfolios in the input datasets.

# [04737] Learning mappings on Wasserstein space with mean-field neural networks

## **Format :** Talk at Waseda University

**Author(s) :** HUYEN PHAM (Université Paris Cité )Xavier Warin (EDF)

**Abstract :** We study the machine learning task for models with operators mapping between the Wasserstein space of probability measures and a space of functions. Two classes of neural networks based on bin density and on

cylindrical approximation, are proposed to learn these so-called mean-field functions, and are theoretically supported by universal approximation theorems. We perform numerical experiments for training these two mean-field neural networks, and show their accuracy in the generalization error with various test distributions.

## [04743] Neural Optimal Stopping Boundary

**Format :** Talk at Waseda University

**Author(s) :** Anders Max Reppen (Boston University Questrom School of Business)Halil Mete Soner (Princeton University)Valentin Tissot-Daguette (Princeton University)

**Abstract :** A method based on deep artificial neural networks and empirical risk minimization is developed to calculate the boundary separating the stopping and continuation regions in optimal stopping. The algorithm parameterizes the stopping boundary as the graph of a function and introduces relaxed stopping rules based on fuzzy boundaries to facilitate efficient optimization. Several financial instruments, some in high dimensions, are analyzed through this method, demonstrating its effectiveness. The existence of the stopping boundary is also proved under natural structural assumptions.

## [05236] MFG-OMO: An optimization framework for mean field game

**Format :** Talk at Waseda University

**Author(s) :** Xin Guo (UC Berkeley)

**Abstract :** We propose a new mathematical paradigm to analyze discrete-time mean-field games. It removes the contractive and the monotone assumptions and the uniqueness of the Nash equilibrium imposed in existing approaches for mean-field games. We show that finding Nash equilibrium solutions for a general class of discrete-time mean-field games is equivalent to solving an optimization problem with bounded variables and simple convex constraints, called MF-OMO. This equivalence framework enables finding multiple (and possibly all) Nash equilibrium solutions of mean-field games by

standard algorithms. For instance, projected gradient descent is shown to be capable of retrieving all possible Nash equilibrium solutions when there are finitely many of them, with proper initializations.

Moreover, analyzing mean-field games with linear rewards and mean-field independent dynamics is reduced to solving a finite number of linear programs, hence solvable in finite time.

Based on joint work with Anran Hu (University of Oxford) and Junzi Zhang (Amazon).

01145 (2/2) : 5C @D505 [Chair: A. Max Reppen]

## [03993] Statistical Learning with Sublinear Regret of Propagator Models

**Format :** Talk at Waseda University

**Author(s) :** Yufei Zhang (London School of Economics and Political Science)Eyal Neuman (Imperial College London)

**Abstract :** We consider a class of learning problems in which an agent liquidates a risky asset while creating both transient price impact driven by an unknown convolution propagator and linear temporary price impact with an unknown parameter. We characterize the trader's performance as maximization of a revenue-risk functional, where the trader also exploits available information on a price predicting signal. We present a trading algorithm that alternates between exploration and exploitation phases and achieves sublinear regrets with high probability. For the exploration phase we propose a novel approach for non-parametric estimation of the price impact kernel by observing only the visible price process and derive sharp bounds on the convergence rate, which are characterised by the singularity of the propagator. These kernel estimation methods extend existing methods from the area of Tikhonov regularisation for inverse problems and are of independent interest. The bound on the regret in the exploitation phase is obtained by deriving stability results for the optimizer and value function of the associated class of infinite-dimensional stochastic control problems.

## [04781] ROBUST UTILITY OPTIMIZATION VIA A GAN APPROACH

**Format :** Talk at Waseda University

**Author(s) :** Hanna Wutte (ETH Zurich)Florian Krach (ETH Zurich)Josef Teichmann (ETH Zurich)

**Abstract :** We study the robust expected utility maximization problem. In this problem, an agent wants to maximize the expected utility of final wealth  $X_T^\pi$  under her trading strategy  $\pi$  in an uncertain market environment that chooses the worst case market measure  $P$  for the given trading strategy, i.e.,  $\sup_\pi \inf_P \mathbb{E}_P[U(X_T^\pi)]$ . This problem can be understood as a two-player zero-sum game between the agent and the market. We restrict our attention to markets consisting of one risk-free and  $d$  risky assets  $S$ . Risky assets  $S$  are given by Itô processes,

where the drift  $\mu$  and diffusion  $\sigma$  are chosen by the market player out of a set of admissible candidate functions. To make this tractable, we consider a penalized version of the robust utility optimization problem, where the market model can choose any such continuous functions, but is penalized for deviating from a reference market model via a penalty functional  $F$ . We suggest an algorithm to solve this problem using two recurrent neural networks (RNNs) with parameters  $\theta$  and  $\omega$ , one for the agent and one for the market, respectively. Those RNNs are trained iteratively by competing in the zero-sum game

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\begin{equation}\sup\{\theta\}\inf\{\omega\}\mathbb{E}[U(X^{\pi_\theta,\mu_\omega,\sigma_\omega})] + F(\mu_\omega,\sigma_\omega,S)\end{equation}
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On a high level, this can be interpreted as a generative adversarial network (GAN) approach, where the generator produces a trading strategy  $\pi_\theta$  and the adversarial discriminator tries to find the worst case market model  $(\mu_\omega, \sigma_\omega)$ . Importantly, the use of RNNs allows both players to learn non-Markovian strategies. The utility function  $U$  as well as the penalty function  $F$  can be chosen freely. We examine several set-ups to empirically show the quality of our proposed algorithm. At first, we consider log-utility in a friction-less market and instantaneous penalization of the market parameters. In this case, an analytic solution is known to exist which is replicated by our trained model. When introducing friction to the market, or when using other utility functions or path-dependent penalties, analytic solutions no longer exist. Therefore, we construct new evaluation metrics and we observe that our trained model achieves convincing results.

This is joint work with Florian Krach and Josef Teichmann.

[05102] Deep Learning in Portfolio Selection under Market Frictions

**Format** : Talk at Waseda University

**Author(s)** : Chen Yang (The Chinese University of Hong Kong)

**Abstract :** Incorporating market frictions in portfolio selection problems often leads to high-dimensionality even when the number of stocks is low, which makes it challenging for traditional grid-based numerical method. In this talk, we explore the application of deep learning method in portfolio selection problems with market frictions such as price impact, transaction cost, and capital gain taxes, and discuss the potential challenges.

## [05342] Machine Learning Surrogates for Parametric and Adaptive Optimal Execution

**Format** : Talk at Waseda University

**Author(s)** : Michael Ludkovski (U California at Santa Barbara) Tao Chen (U of Michigan) Moritz Voss (U California at Los Angeles)

**Abstract :** We investigate optimal order execution with dynamic parametric uncertainty. Our base model features discrete time, stochastic transient price impact generalizing Obizhaeva and Wang (2013). We first consider learning the optimal strategy across a multi-dimensional range of model configurations, including price impact and resilience parameters, as well as initial stochastic states. We develop a numerical algorithm based on dynamic programming and deep learning, utilizing an actor-critic framework to construct two neural-network (NN) surrogates for the value function and the feedback control. We then apply the lens of adaptive robust stochastic control to consider online statistical learning of model parameters along with a worst-case min-max optimization. Thus, the controller is dynamically learning model parameters based on her observations while explicitly accounting for Bayesian uncertainty of the learned parameter estimates. We propose a modeling framework which allows a time-consistent 3-way marriage between dynamic learning, dynamic robustness and dynamic control. We extend our NN approach to tackle the resulting 8-dimensional adaptive robust optimal order execution problem, and illustrate with comparisons to alternative frameworks, such as adaptive or static robust strategies.

# [01149] Sparse optimization techniques and applications

**Session Time & Room** : 4E (Aug.24, 17:40-19:20) @D515

**Type :** Proposal of Minisymposium

**Abstract :** Natural data that arise in several applications (such as biomedical imaging) are inherently sparse in suitable transformation domains provided in general by the gradient, wavelets, and their other variants. Such data sets can be stored in terms of a few samples, which in turn can be used for retrieving the original data with minimal or no loss of information via sparsity-seeking optimization techniques. A wealth of recent developments -

going by the name of compressive sensing - aim at signal acquisition compressively and sparse (or economical) description of data of certain types. Of late, this area of research has seen some fascinating developments, which include adaptive solvers, sparsity-driven deep learning methods, hardware-friendly algorithms suitable for biomedical imaging and impedance tomography, etc. The symposium aims at discussing some recent developments in sparse representation/optimization theory that pertain to fundamental as well as application-centric topics.

**Organizer(s)** : K. Z. Najiya, R. Ramu Naidu, Pradip Sasimal, Phanindra Jampana

**Classification** : 92C55

**Minisymposium Program :**

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01149 (1/1) : 4E @D515 [Chair: PRADIP SASMAL]

## [05057] Efficient Magnetic Resonance Imaging via Adaptive Sparse Optimization

**Format** : Online Talk on Zoom

**Author(s)** : NAJIYA K Z (Post Doctoral Fellow)

**Abstract** : Magnetic resonance imaging via compressed sensing techniques gives good-quality reconstructions due to the sparse nature of images in the gradient domain. In routine medical scanning scenarios, the consecutive MRI images need not differ much in general. In this talk, we explain an MR imaging technique via sparse minimization by incorporating additional information about the support estimate into the optimization process to recover images from a lesser number of measurements.

## [05058] A new matrix factorization for sparse representation of over-determined systems

**Format** : Talk at Waseda University

**Author(s)** : NAJIYA K Z (PhD Scholar)C S Sastry (IIT Hyderabad)

**Abstract** : This presentation aims at discussing a novel method that finds a sparse approximation of a matrix system  $y = Ax$  (where  $A$  has a bigger row size compared to its column size). While highlighting the need for such an approximation through some applications, the presentation realizes its objective via a new matrix factorization. Besides, it compares and contrasts the proposed method with established ones that have similar objectives.

## [05060] Sparse optimization-based ERT algorithms for multiphase flows

**Format** : Talk at Waseda University

**Author(s)** : NAJIYA K Z (PhD Scholar)Shantanu Gulati (IIT Hyderabad)

**Abstract** : We discuss applications of the compressed sensing framework mainly in the field of Electrical Impedance tomography (EIT). EIT is a scanning technique that draws a relationship between the impedance inside the domain and the current to voltage map on the boundary at the electrodes. In particular, we wish to address the ill-posed inverse problem in the circular domain. The idea is to draw comparisons and improve upon the existing techniques with L 1 and the weighted-norm approaches.

## [05061] Hardware-friendly binary frames for sparse optimization

**Format** : Talk at Waseda University

**Author(s)** : NAJIYA K Z (PhD Scholar)Prasad Theeda (Vellore Institute of Technology)

**Abstract** : Binary matrices are preferred as compressed sensing (CS) matrices because they are hardware-friendly and support low-complexity sparse recovery algorithms. In this talk, we discuss that the disjunctness property of a binary matrix, which has been used in non-adaptive group testing, can also be very useful for recovering sparse signals. Disjunct matrices are particularly well-suited as compressed sensing matrices because they can support a non-iterative, fast sparse recovery algorithm.

# [01152] Recent trends in the mathematical theory for incompressible fluids

**Session Time & Room :**

01152 (1/3) : 4E (Aug.24, 17:40-19:20) @G703

01152 (2/3) : 5B (Aug.25, 10:40-12:20) @G703

01152 (3/3) : 5C (Aug.25, 13:20-15:00) @G703

**Type :** Proposal of Minisymposium

**Abstract :** Models for incompressible fluid flows are omnipresent in a.o. (geo-)physical, biological and engineering applications. Nonetheless, the intrinsic lack of regularity of solutions to systems such as the incompressible Euler and Navier-Stokes equations constitutes a central challenge in developing further their mathematical theory.

The mini-symposium approaches these regularity questions from both a deterministic and stochastic perspective with a focus on most recent results on singularity formation, regularization procedures, the emergence of quasi-periodic solutions and hydrodynamic stability.

We bring together speakers from diverse backgrounds in terms of region, gender, and specific research methods to foster and encourage scientific exchange between different communities.

**Organizer(s) :** Gennaro Ciampa, Lars Eric Hientzsch

**Classification :** 35Q35, 35Q31, 76B03, 76F02, 76B47

**Minisymposium Program :**

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01152 (1/3) : 4E @G703 [Chair: Lars Eric Hientzsch]

## [03906] Geometric structures in incompressible fluids: vortex and magnetic reconnection

**Format :** Talk at Waseda University

**Author(s) :** Gennaro Ciampa (University of Milan)

**Abstract :** The goal of this talk is to provide examples of smooth solutions of the Navier-Stokes equations such that the topology of the vortex lines changes during the evolution without any loss of regularity. This phenomenon is known as vortex reconnection. We will also discuss the applications to Magnetohydrodynamics: we will construct smooth solutions of the MHD equations such that the topology of the magnetic field lines changes during evolution, providing analytical examples of magnetic reconnection.

## [04219] On maximally mixed equilibria of two-dimensional perfect fluid

**Format :** Talk at Waseda University

**Author(s) :** Michele Dolce (EPFL)

**Abstract :** The motion of a 2D perfect fluid can be described as an area-preserving rearrangement of the initial vorticity that conserves the kinetic energy. In the infinite time limit, vorticity mixing can occur and is conjectured to be a generic phenomenon. We offer a new perspective on the "maximally mixed states" introduced by Shnirelman by proving that many of them can be obtained as minimizers of a variational problem and we discuss some of their properties.

## [03417] Quasi-periodic invariant structures in incompressible fluids

**Format :** Talk at Waseda University

**Author(s) :** Luca Franzoi (New York University Abu Dhabi)Nader Masmoudi (New York University Abu Dhabi)RICCARDO MONTALTO (University of Milan)

**Abstract :** In this talk, I present a recent result about the existence of nontrivial steady flows near the Couette flow in the channel  $\mathbb{R} \times [-1, 1]$  that are quasi-periodic in space and solve the incompressible Euler equations.

First, I recall the result of Lin & Zeng and their construction of periodic flows. Then, I state the main result for space quasi-periodic flows. Finally, I show what are the main issues in our construction and how to solve them.

## [03123] Flows with lower dimensional dissipations

**Format :** Online Talk on Zoom

**Author(s) :** Luigi De Rosa (University of Basel)

**Abstract :** In my talk I will describe how to put in a rigorous framework the study of turbulent solutions, i.e. rough fluid flows, whose energy cascade accumulates on lower dimensional sets. This naturally connects to intermittency phenomena which have been playing a major role in the current mathematical research.

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01152 (2/3) : 5B @G703 [Chair: Luca Franzoi]

## [03363] Uniform in gravity estimates for 2D water waves

**Format :** Talk at Waseda University

**Author(s) :** Siddhant Agrawal (ICMAT)

**Abstract :** We consider the 2D gravity water waves equation on an infinite domain. We prove a local wellposedness result which allows interfaces with corners and cusps as initial data, such that the time of existence of solutions is uniform even as the gravity parameter  $g \rightarrow 0$ . As an application of the new energy estimate, we prove a blow up result for the water waves model where the fluid is homeomorphic to the disc.

## [04740] Invariant KAM tori around annular vortex patches for 2D Euler equations

**Format :** Talk at Waseda University

**Author(s) :** Zineb Hassainia (NYUAD)Taoufik Hmidi (New York University Abu Dhabi)Emeric Roulley (SISSA International School for Advanced Studies)

**Abstract :** We shall discuss the emergence of quasi periodic vortex patch solutions with one hole for the 2D-Euler equations. We prove the existence of such structures close to any annular vortex patch provided that its modulus belongs to a Cantor set with almost full Lebesgue measure. The proof is based on Nash-Moser implicit function theorems and KAM theory.

## [03663] Euler and Navier-Stokes equations. Quasi-periodic solutions and inviscid limit

**Format :** Talk at Waseda University

**Author(s) :** RICCARDO MONTALTO (University of Milan)

**Abstract :** In this talk I will discuss some recent results on Euler and Navier Stokes equations concerning the construction of quasi-periodic solutions. In particular, I will focus on the construction of vanishing viscosity quasi-periodic solutions for the Navier-Stokes equation in the inviscid limit. The key step of the analysis is to implement Normal Form techniques which allow to prove sharp estimates (uniform in time) w.r. to the viscosity.

## [04625] Reducibility of a class of quasi-linear wave equation on the torus

**Format :** Talk at Waseda University

**Author(s) :** Shulamit Terracina (Università degli Studi di Milano)

**Abstract :** We discuss the reducibility of a linear wave equation on the torus perturbed by a pseudo-differential potential of order 2 depending quasi-periodically on time. Under suitable conditions on the frequency vector, we develop a general strategy, combining Egorov theory with straightening of vector fields, to reduce to constant coefficients a class of weakly dispersive operators. Finally, we discuss generalizations to operators arising from the linearization of fluid models such as pure gravity Water Waves.

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01152 (3/3) : 5C @G703 [Chair: Gennaro Ciampa]

## [02208] Nonuniqueness in Law for Stochastic Hypodissipative Navier--Stokes Equations

**Format :** Talk at Waseda University

**Author(s) :** Andre Schenke (Courant Institute of Mathematical Sciences at New York University)

**Abstract :** We study the incompressible hypodissipative Navier--Stokes equations with dissipation exponent  $0 < \alpha < \frac{1}{2}$  on the three-dimensional torus perturbed by an additive Wiener noise term and prove the existence of an initial condition for which distinct probabilistic weak solutions exist. To this end, we employ convex integration

part\_2

methods to construct a pathwise probabilistically strong solution, which violates a pathwise energy inequality up to a suitable stopping time. This paper seems to be the first in which such solutions are constructed via Beltrami waves instead of intermittent jets or flows in a stochastic setting.

### [02509] Restoration of well-posedness of 2D fluid dynamics equations by transport noise

**Format :** Talk at Waseda University

**Author(s) :** Lucio Galeati (EPFL)Dejun Luo (Academy of Mathematics and Systems Science, Chinese Academy of Sciences)

**Abstract :** A longstanding problem in fluid dynamics is whether solution to 2D Euler with  $L^p$ -valued vorticity are unique, for some  $p < \infty$ . A related question on the probabilistic side is whether one can find a physically meaningful noise that can restore such uniqueness. Here I will present some recent progress, concerning other closely related 2D equations, for which we can provide a positive answer. Based on a joint work with Dejun Luo.

### [04785] Finite-time blowup for a 3D hypo-dissipative Navier-Stokes model equation

**Format :** Talk at Waseda University

**Author(s) :** Evan Miller (University of British Columbia)

Johannes Haubner (University of Graz)

Bastian Zapf (University of Oslo)

**Abstract :** In this talk, I will discuss a new blowup result for a model equation for the 3D hypo-dissipative Navier-Stokes equation based on considering a restricted constraint space. When imposing the right geometric conditions on initial data, involving planar stretching at the origin, this allows a forward energy cascade that generates finite-time blowup. This model equation respects both the energy equality and the identity for enstrophy growth.

### [05631] Nonlinear Landau damping for the Vlasov-Poisson system in the whole space around Penrose-stable equilibria

**Author(s) :** Quoc Hung Nguyen (Academy of Mathematics and Systems Science,)Lingjia Huang (Fudan University, Shanghai)

**Abstract :** In this talk, will present recent results on the nonlinear asymptotic stability of the stable equilibria among solutions of the Vlasov Poisson system in  $\mathbb{R}^2$  and  $\mathbb{R}^3$ .

## [01158] Oblique derivative boundary volume problems - numerical methods and applications

**Session Time & Room :** 4C (Aug.24, 13:20-15:00) @E506

**Type :** Proposal of Minisymposium

**Abstract :** In this mini-symposium we will focus on recent efforts in developing various numerical approaches for solving the oblique derivative boundary volume problems. Namely, we will apply the finite element, finite volume and boundary element methods to solve different engineering problems which involve the oblique derivatives.

**Organizer(s) :** Marek Macák, Zuzana Minarechová

**Classification :** 65N30, 35Q86, 65N08

**Minisymposium Program :**

01158 (1/1) : 4C @E506

## [02007] The finite element method for solving the oblique derivative boundary value problems in geodesy

**Author(s)** : Marek Macák (Slovak University of Technology) Zuzana Minarechová (Slovak University of Technology) Karol Mikula (Slovak University of Technology) Robert Cunderlik (Slovak University of Technology)

**Abstract** : We present approach to approximate the solution of the Laplace equation with an oblique derivative boundary condition by the finite element method. For this approach we perform testing experiments to study its behaviour and convergence. Finally, the usefulness of this approach is demonstrated by using it to gravity field modelling, namely, to approximate the solution of a geodetic boundary value problem in Himalayas.

## [02121] Curvature and Torsion of Gravitational Plumb Lines

**Author(s)** : Zhi Yin (Jiangsu Ocean University) Nico Smeuw (University of Stuttgart) Keifei Zhang (China University of Mining and Technology)

**Abstract** : In our previous research, we reformulate the gravitational field in terms of a potential flow; the gravitational vector field is mapped onto a potential-flow velocity field, in which the plumb line and the stream line are equivalent to each other. Here, we further investigate the curvature and the torsion of a gravitational plumb line by utilizing the fundamental equations of the potential flow. We expect them to have a good practical application in exploration geophysics.

## [02131] The finite volume method for solving the oblique derivative BVP in geodesy

**Author(s)** : Zuzana Minarechová (Slovak University of Technology) Marek Macák (Slovak University of Technology) Karol Mikula (Slovak University of Technology) Róbert Čunderlik (Slovak University of Technology)

**Abstract** : We formulate the oblique derivative boundary value problem applied in gravity field and present two approaches to its solution by the finite volume method. In the first approach, the oblique derivative in the boundary condition is decomposed into normal and two tangential components and approximated by the central scheme. In the second approach, the oblique derivative in the boundary condition is treated by the first order upwind scheme. Both approaches are tested by various experiments.

## [02887] Finite Volume Approximate Solutions of Some Oblique Derivative Boundary Value Problems and Applications

**Author(s)** : Abdallah BRADJI (University of Annaba-Algeria)

**Abstract** : In this work, we review previous works on FVMs (Finite Volume methods) for Elliptic and Parabolic equations with oblique derivatives boundary conditions. We start by the first two works with Gallouet (Aix-Marseille University, France) which dealt with FV on the so-called Admissible meshes for Elliptic equations.

We subsequently describe our work with Fuhrmann (WIAS, Berlin-Germany) which dealt with FV using the nonconforming meshes and the SUSHI for Elliptic and Parabolic equations with oblique derivatives boundary conditions.

Finally, we focus on FVMs for Elliptic equations with mixed oblique boundary equations and application to Inverse Problems. This work is done jointly with Lesnic (Leeds University, UK).

We sketch at the end some works, related to the subject, which are in progress.

## [01161] Error-Controlled Adaptive Algorithms in Full-Order and Reduced-Order Model Simulations

**Session Time & Room** : 1C (Aug.21, 13:20-15:00) @E604

**Type** : Proposal of Minisymposium

**Abstract** : Controlling numerical errors is of high importance in simulation of various science and engineering problems, e.g., solids, fluids, and air. In full-order model simulations, the discretization error between the continuous solution and the discrete one plays a central role. In reduced-order model simulations, approximation errors during the reduction process is pivotal. Recent research advancements in both these domains have been on

development of error-controlled adaptive algorithms, which is the focus of this minisymposium.

**Organizer(s)** : Kapil Ahuja, Marc C. Steinbach, and Thomas Wick

**Classification** : 65Fxx, 65Gxx, 65Lxx, 41A05, 34C20, Error Control, Model Order Reduction, Finite Element Method

**Minisymposium Program :**

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01161 (1/1) : 1C @E604 [Chair: Bernhard Endtmayer]

## [01786] Modeling and multigoal-oriented a posteriori error control for heated material processing using a generalized Boussinesq modell

**Format** : Talk at Waseda University

**Author(s)** : Sven Beuchler (IfAM, Leibniz University Hanover)Bernhard Endtmayer (IfAM, Leibniz University Hanover)Johannes Lankeit (IfAM, Leibniz University Hanover)Thomas Wick (IfAM, Leibniz University Hanover)

**Abstract** : In this presentation, we develop a posteriori error control for a generalized Boussinesq model. The stationary Navier-

Stokes equations with temperature dependent viscosity are coupled with a stationary heat equation. We use the dual-weighted residual method in which an adjoint problem is utilized to obtain sensitivity measures with respect to several goal functionals. The error localization is done with the help of a partition-of-unity in a weak formulation. The resulting error estimators are used within an adaptive algorithm. Finally, numerical examples are presented.

## [04451] Error-Controlled Local Interpolation of Moment Matching Reduced Order Models for Vibroacoustics

**Format** : Talk at Waseda University

**Author(s)** : Harikrishnan K. Sreekumar (Technische Universität Braunschweig, Institut für Akustik)Ulrich Römer (Technische Universität Braunschweig, Institut für Dynamik und Schwingungen)Matthias Bollhöfer (Technische Universität Braunschweig, Institut für Numerische Mathematik)Christopher Blech (Technische Universität Braunschweig, Institut für Akustik)Sabine C. Langer (Technische Universität Braunschweig, Institut für Akustik)

**Abstract** : Surrogate modeling for high-dimensional parametric problems is computationally challenging and therefore demands techniques to capture the essential features with the least effort. To this end, we present an adaptive error-controlled strategy to drive accurate modeling at two levels: moment matching reduced-order models approximating the frequency response and sparse grid interpolation for parametric approximation. We compare dimension-adaptive and spatially-adaptive refinement strategies with respect to convergence, demonstrated using problems from vibroacoustics.

## [04671] Advances in A Posteriori Error Estimation and Adaptive Model Order Reduction

**Format** : Talk at Waseda University

**Author(s)** : Sridhar Chellappa (Max Planck Institute for Dynamics of Complex Technical Systems, Magdeburg)Lihong Feng (Max Planck Institute for Dynamics of Complex Technical Systems, Magdeburg)Peter Benner (MPI for Dynamics of Complex Technical Systems, Magdeburg)

**Abstract** : Reduced-order models (ROMs) play an important role in applications such as engineering design, control, optimization, etc. which require reliable simulations of large-scale systems in real-time. We discuss our recent work on a posteriori error estimation and adaptivity. The objective of this work is to reduce the training cost for ROM. We discuss several new error estimators and illustrate their use in adaptive basis enrichment and adaptive parameter sampling. The benefits of the adaptive methods are demonstrated on several numerical examples.

## [05257] Stable Linear Solves in Parametric Model Order Reduction

**Format** : Online Talk on Zoom

**Author(s)** : Kapil Ahuja (Indian Institute of Technology Indore (IIT Indore))Navneet Pratap Singh (Bennett University)

**Abstract** : We study stability of class of algorithms for model order reduction (MOR) of parametric linear dynamical systems, with respect to inexact linear solves. Our most novel contribution is achieving backward stable MOR algorithms. To achieve this, we first adapt the underlying linear solver such that it satisfies orthogonalities

required for stability. Next, we demonstrate that by suitably using a recycling variant of the solver, these orthogonalities can be satisfied without any code changes and cheaply.

## [01165] Adapted Wasserstein distance for robust finance

**Session Time & Room :** 5D (Aug.25, 15:30-17:10) @D505

**Type :** Proposal of Minisymposium

**Abstract :** The minisymposium brings together scientists working on the developments of new transport distances suited for the analysis of financial markets in case of model uncertainty. The four talks illustrate the powerful use of newly

developed tools in optimal transport, and in particular of the Adapted Wasserstein distance, to tackle crucial problems in finance, such as robustness of optimal decision making to model misspecification.

**Organizer(s) :** Beatrice Acciaio  
**Sponsor :** This session is sponsored by the SIAM Activity Group on Financial Mathematics and Engineering.

**Classification :** 91G80, 49Q22

**Minisymposium Program :**

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01165 (1/1) : 5D @D505 [Chair: Beatrice Acciaio]

### [05605] Adapted Wasserstein distance for model-uncertainty in finance

**Format :** Talk at Waseda University

**Author(s) :** Beatrice Acciaio (ETH Zurich)

**Abstract :** I will illustrate the suitability of adapted transport distances in the context of model-uncertainty in finance. I will then present two consistent estimators for the Adapted Wasserstein distance, showing that we can recover the optimal rates of the classical empirical measure with respect to Wasserstein distance.

### [05606] Adapted Wasserstein distance between the laws of SDEs

**Format :** Talk at Waseda University

**Author(s) :** Beatrice Acciaio (ETH Zurich)Sigrid Kallblad (KTH Royal Institute of Technology in Stockholm)

**Abstract :** We consider here an adapted optimal transport problem between the laws of Markovian stochastic differential equations (SDEs) and establish optimality of the so-called synchronous coupling between the given laws. The proof of this result is based on time-discretisation methods and reveals an interesting connection between the synchronous coupling and the celebrated discrete-time Knothe–Rosenblatt rearrangement. We also provide a result on equality of various topologies when restricting to certain types of laws of continuous-time processes. The talk is based on joint work with Julio Backhoff and Ben Robinson.

### [05607] Adapted Wasserstein distance on the space of continuous time stochastic processes.

**Format :** Talk at Waseda University

**Author(s) :** Beatrice Acciaio (ETH Zurich)Xin Zhang (University of Vienna)

**Abstract :** Stochastic processes are often used as models for stock prices, and people were interested in the stability of optimal stopping problem in Finance with respect to the underlying model. We define the adapted Wasserstein distance on the space of stochastic processes, which is an extension of the usual Wasserstein distance between laws of stochastic processes. We prove that the optimal stopping problem is continuous with respect to the resulting topology, Martingales form a closed subset and approximation results like Donsker's theorem extend to the adapted Wasserstein distance.

## [05608] On concentration of the empirical measure for general transport costs

**Format :** Talk at Waseda University

**Author(s) :** Beatrice Acciaio (ETH Zurich)Johannes Wiesel (CMU)

**Abstract :** Let  $\mu$  be a probability measure on  $\mathbb{R}^d$  and  $\mu_N$  its empirical measure with sample size  $N$ . We prove a concentration inequality for the optimal transport cost between  $\mu$  and  $\mu_N$  for cost functions with polynomial local growth, that can have superpolynomial global growth. This result generalizes and improves upon estimates of Fournier and Guillin. By partitioning  $\mathbb{R}^d$  into annuli, we infer a global estimate from local estimates on the annuli and conclude that the global estimate can be expressed as a sum of the local estimate and a mean-deviation probability for which efficient bounds are known. This talk is based on joint work with Martin Larsson and Jonghwa Park.

## [01167] Recent development in mean field control and learning

**Session Time & Room :**

01167 (1/2) : 1E (Aug.21, 17:40-19:20) @F403

01167 (2/2) : 2C (Aug.22, 13:20-15:00) @F403

**Type :** Proposal of Minisymposium

**Abstract :** Mean field control problems have attracted massive interest and provide a promising approach dealing with multi-agent systems. The aim of this mini-symposium is to share the new trends of both theory and applications of this area. We would like to invite the frontier scholars to talk about recent developments in various learning methods for the mean field control problems under different application aspects, as well as analyzing HJB equation in the infinite dimensional spaces for the theory prospective.

**Organizer(s) :** Xin Guo, Jiacheng Zhang  
**Sponsor :** This session is sponsored by the SIAM Activity Group on Financial Mathematics and Engineering.

**Classification :** 49N80, 35Q89

**Minisymposium Program :**

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01167 (1/2) : 1E @F403 [Chair: Jiacheng Zhang]

## [04658] Actor-critic learning for mean-field control in continuous time

**Format :** Talk at Waseda University

**Author(s) :** HUYEN PHAM (Université Paris Cité )Noufel Frikha (Université Paris 1)Maximilien Germain (Morgan Stanley )Mathieu Laurière (NYU Shanghai)Xuanye Song (Université Paris Cité )

**Abstract :** We study policy gradient for mean-field control in continuous time in a reinforcement learning setting. By considering

randomised policies with entropy regularisation, we derive a gradient expectation representation of the value function, which is amenable to actor-critic type algorithms, where the value functions and the policies are learnt alternately

based on observation samples of the state and model-free estimation of the population state distribution, either by offline or online learning.

## [04674] Mean-field singular control problem: regularity and related mean-field reflected diffusion

**Format :** Talk at Waseda University

**Author(s) :** Jodi Dianetti (Bielefeld University)Xin Guo (UC Berkeley)Jiacheng Zhang (UC Berkeley)Huyê Pham (Université Paris Cité )

**Abstract :** We study a class of mean-field control problems with singular controls. Such a model represents the limit of the control problems in which a controller can adjust, through a bounded variation process, an underlying diffusion, which in turn affects an n-particle system. Adopting appropriate notions of convexities, we are able to establish the regularity of the value function of the problem and to show the existence of the optimal control. The

regularity of the value function allows to characterize the solution of the problem in terms of a related mean-field Skorokhod problem. This consists in keeping the optimally controlled state process in a region prescribed by the derivative of the value function, by using the optimal control in order to reflect the state at its boundary.

## [04752] A non-asymptotic perspective on mean field control

**Format :** Talk at Waseda University

**Author(s) :** Lane Chun Yeung (Columbia University) Daniel Lacker (Columbia University) Sumit Mukherjee (Columbia University)

**Abstract :** We study a class of stochastic control problems in which a large number of players cooperatively choose their drifts to maximize an expected reward minus a quadratic running cost. For a broad class of potentially asymmetric rewards, we show that there exist approximately optimal controls which are decentralized, in the sense that each player's control depends only on its own state and not the states of the other players.

## [05079] Signature SDEs with jumps and their tractability properties

**Format :** Talk at Waseda University

**Author(s) :** Christa Cuchiero (University of Vienna) Francesca Primavera (University of Vienna) Sara Svaluto Ferro (University of Verona)

**Abstract :** Signature-based models have recently entered the field of Mathematical Finance. Relying on recent advances on the signature of càdlàg paths, we introduce here a generic class of jump-diffusion models via so-called signature SDEs with jumps. We elaborate on their tractability properties and show that the signature-based models for asset prices proposed so far can be embedded in this framework. As a special case, we focus on jump-diffusions with entire characteristics, leading to a far-reaching extension of the class of polynomial processes.

01167 (2/2) : 2C @F403 [Chair: Jiacheng Zhang]

## [05419] Markov $\alpha$ -Potential Game

**Format :** Online Talk on Zoom

**Author(s) :** Xinyu Li (UC Berkeley) Xin Guo (UC Berkeley) Chinmay Maheshwari (UC Berkeley) Manxi Wu (Cornell University) Shankar Sastry (UC Berkeley)

**Abstract :** We propose a new framework to study multi-agent interaction in Markov games: Markov  $\alpha$ -potential games. Markov potential games are special cases of Markov  $\alpha$ -potential games, so are two important and practically significant classes of games: Markov congestion games and perturbed Markov team games. In this paper,  $\alpha$ -potential functions for both games are provided and the gap  $\alpha$  is characterized with respect to game parameters. Two algorithms – the projected gradient-ascent algorithm and the sequential maximum improvement smoothed best response dynamics – are introduced for approximating the stationary Nash equilibrium in Markov  $\alpha$ -potential games. The Nash-regret for each algorithm is shown to scale sub-linearly in time horizon. Our analysis and numerical experiments demonstrates that simple algorithms are capable of finding approximate equilibrium in Markov  $\alpha$ -potential games.

## [05421] MF-OMO: An Optimization Formulation of Mean-Field Games

**Format :** Online Talk on Zoom

**Author(s) :** Xin Guo (UC Berkeley) Anran Hu (University of Oxford) Junzi Zhang (Citadel Securities)

**Abstract :** The literature on theory and computation of mean-field games (MFGs) has grown exponentially recently, but current approaches are limited to contractive or monotone settings, or with an a priori assumption of the uniqueness of the Nash equilibrium (NE). In this talk, we present MF-OMO (Mean-Field Occupation Measure Optimization), a mathematical framework that analyzes MFGs without these restrictions. MF-OMO reformulates the problem of finding NE solutions in MFGs as a single optimization problem. This formulation thus allows for directly utilizing various optimization tools, algorithms and solvers to find NE solutions of MFGs in practice. We also provide convergence guarantees for finding (multiple) NE solutions using popular algorithms like projected gradient descent. For MFGs with linear rewards and mean-field independent dynamics, solving MF-OMO can be reduced to solving a finite number of linear programs, hence solved in finite time.

## [05439] The convergence problem in mean field control

**Format :** Online Talk on Zoom

**Author(s) :** Joe Jackson (The University of Texas at Austin)Samuel Daudin (Université Côte d'Azur) François Delarue (Université Côte d'Azur)

**Abstract :** This talk will be about a recent joint work with Samuel Daudin and François Delarue concerning the convergence problem in mean field control. When the data is convex and sufficiently smooth, the (optimal) rate of convergence (of the  $N$ -player value function towards the limiting value function) is known to be  $1/N$ . The goal of our work is to identify the optimal rate of convergence in the more subtle non-convex setting.

## [01168] Network based reduced-order models for forward and inverse PDE problems

**Session Time & Room :**

01168 (1/2) : 5B (Aug.25, 10:40-12:20) @E711

01168 (2/2) : 5C (Aug.25, 13:20-15:00) @E711

**Type :** Proposal of Minisymposium

**Abstract :** Reduced order models (ROMs) have been proven to be a powerful and versatile tool for a fast and robust large-scale simulations as well as imaging and inversion. In this minisymposium we will focus on a special class of ROMs, network-based ROMs, that originate from network synthesis. It allows to represent ROM in terms of sparsely-connected networks and enables a direct physical interpretation. We shall discuss various techniques to construct such ROMs as well as their applications.

**Organizer(s) :** Vladimir Druskin, Alexander Mamonov, Mikhail Zaslavskiy

**Classification :** 65R32, 65N21, 65M99, reduced-order models, inverse scattering problems, large-scale forward problems

**Minisymposium Program :**

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01168 (1/2) : 5B @E711 [Chair: Alexander Mamonov]

## [02869] Regularized Lippmann-Schwinger-Lanczos Algorithm for Inverse Scattering Problems in the Frequency Domain

**Format :** Talk at Waseda University

**Author(s) :** Justin Baker (University of Utah)Elena Cherkaev (University of Utah)Vladimir Druskin (Worcester Polytechnic Institute)Shari Moskow (Drexel University)Mikhail Zaslavsky (Schlumberger-Doll Research Center)

**Abstract :** Inverse scattering techniques have broad applicability in medical imaging, geophysics, and remote sensing. This talk presents a robust direct reduced order model (ROM) method for solving inverse scattering problems. The approach is based on a Lippmann-Schwinger-Lanczos (LSL) algorithm in the frequency domain with two levels of regularization. Results of numerical experiments for Schrödinger and Helmholtz problems show that the proposed regularization scheme significantly improves the performance of the LSL algorithm, allowing for good reconstructions with noisy data.

## [04821] Can one identify damped Stieltjes string from its spectral function?

**Format :** Talk at Waseda University

**Author(s) :** Vladimir Druskin (WPI)Jörn Zimmerling (Uppsala University)Rob Remis (Delft University of Technology)

**Abstract :** The Stieltjes strings were introduced by Gantmakher and Krein as isomorphic mechanical representations of the Stieltjes spectral functions. However, dissipative strings cannot be uniquely identified for the continuous spectral functions, corresponding to the unbounded domains. Generally, any passive transfer function can be represented as a Stieltjes function, that yields a wide class of equivalent solutions. We analyze constraints

leading to the uniqueness for damped problems and numerical implementation in the data-driven ROM framework.

## [04751] Inverse scattering in attenuating media -- a ROM approach

**Format :** Talk at Waseda University

**Author(s) :** Jörn Zimmerling (Uppsala University)Vladimir Druskin (WPI)Rob Remis (TU Delft)

**Abstract :** Inverse scattering problems in attenuating media arise in important applications in biomedical imaging or radar imaging. In inverse scattering the goal is to reconstruct the coefficients of a PDE based on remote measurements of scattered waves. Based on these measurements a reduced-order model can be constructed that goes beyond the typical data fitting. It has a special algebraic structure that allows analogies to finite-difference discretization of PDEs and facilitates efficient solution of the inverse problem.

01168 (2/2) : 5C @E711 [Chair: Vladimir Druskin]

## [05171] REDUCED ORDER MODELING INVERSION OF MONOSTATIC DATA IN A MULTI-SCATTERING ENVIRONMENT

**Format :** Talk at Waseda University

**Author(s) :** Mikhail Zaslavskiy (Southern Methodist University)

**Abstract :** We consider the reduced order model approach for inversion in the monostatic formulation targeting the synthetic aperture radar (SAR) data in the time domain. The monostatic data is given as a series of single input/single output (SISO) responses due to moving collocated sources and receivers, that is, the diagonal of the matrix-valued MIMO transfer matrix. The ROMs are constructed to match the data for each source-receiver pair separately, and these are used to construct internal solutions for the corresponding source using only data-driven Gramian. The data from different locations is then coupled via the approximate Lippman-Schwinger integral equation. Numerical experiments illustrating the performance of our approach will be provided.

## [05531] Waveform Inversion via Reduced Order Modeling

**Format :** Talk at Waseda University

**Author(s) :** Alexander Mamonov (University of Houston)Liliana Borcea (University of Michigan)Josselin Garnier (Ecole Polytechnique)Jörn Zimmerling (Uppsala University)

**Abstract :** We propose a novel approach to full waveform inversion (FWI), based on a data driven reduced order model (ROM) of the wave equation operator. The unknown medium is probed with pulses and the time domain pressure waveform data is recorded on an active array of sensors. The ROM is a projection of the wave equation operator on a subspace of wave equation solution snapshots. It can be constructed from the measured data via a nonlinear process and subsequently used for efficient velocity estimation. While the conventional FWI via nonlinear least-squares data fitting is challenging without low frequency information, and prone to getting stuck in local minima (cycle skipping effect), minimization of ROM misfit is behaved much better, even for a poor initial guess. For low-dimensional parametrizations of the unknown velocity the ROM misfit function is demonstrably close to convex. The proposed approach consistently outperforms conventional FWI in standard synthetic tests, as shown in the numerical experiments.

## [05544] Correlation-informed dictionary learning for imaging in complex media

**Format :** Talk at Waseda University

**Author(s) :** Alexei Novikov (Penn State University)

**Abstract :** We propose an approach for imaging in strongly scattering media that uses dictionary learning and connectivity information to estimate the sensing matrices in these media. It has two steps. The first step estimates, with high accuracy, the true Green's function vectors using array data from multiple sparse sets of sources, whose locations and amplitudes are not known to us. This step yields a dictionary for wave propagation whose columns are those of the sensing matrix up to permutations. The second step orders these columns using Multi-Dimensional Scaling (MDS) with connectivity information derived from cross-correlations of the estimated Green's function vectors. For these two steps to work together, we must combine data from large and small arrays. Through simulation experiments, we show that the proposed approach is robust and is able to provide high-resolution images.

# [01170] High Performance Multigrid Methods for Large-Scale Applications

## **Session Time & Room :**

01170 (1/3) : 5B (Aug.25, 10:40-12:20) @E708

01170 (2/3) : 5C (Aug.25, 13:20-15:00) @E708

01170 (3/3) : 5D (Aug.25, 15:30-17:10) @E708

**Type :** Proposal of Minisymposium

**Abstract :** Multigrid methods are an optimal computational complexity linear solver and preconditioner that is often utilized to solve large-scale problems. The purpose of this minisymposium is to bring together researchers working on high-performance multigrid solvers. The presentations include topics on both performance aspects, advanced architectures, and applications.

**Organizer(s) :** Graham Harper, Peter Ohm

**Classification :** 65Mxx, 65Nxx, 65Fxx, 65Yxx, 65Zxx

## **Minisymposium Program :**

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01170 (1/3) : 5B @E708 [Chair: Graham Harper]

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01170 (2/3) : 5C @E708 [Chair: Peter Ohm]

# [03275] Block-structured and hierarchical hybrid grid matrix-free multigrid solvers for CFD applications at scale

**Format :** Talk at Waseda University

**Author(s) :** Harald Koestler (Friedrich-Alexander Universität Erlangen-Nürnberg)

**Abstract :** In this talk an overview of applications and performance for matrix-free multigrid solvers implemented in the HPC software frameworks HyTeG and ExaStencils is provided. This includes scaling and efficiency results on CPU and GPU clusters and sample applications from geophysics, charged particle and ocean simulations.

# [03867] Performance improvements of algebraic multigrid algorithms on modern system architectures

**Format :** Talk at Waseda University

**Author(s) :** Luc Berger-Vergiat (Sandia National Laboratories) Jonathan Hu (Sandia National Laboratories) Christian Glusa (Sandia National Laboratories) Chris Siefert (Sandia National Laboratories)

**Abstract :** Multigrid methods are an important class of linear solvers and preconditioners for their high scalability on large computing systems. Implementing these algorithms on GPU based platforms remains a challenging task. In this talk we will discuss the current state of the MuLu package of Trilinos which provides algebraic multigrid methods on CPUs and GPUs and present results gathered on recent architectures.

# [03020] Improving AMG Strength of Connection

**Format :** Talk at Waseda University

**Author(s) :** Wayne Mitchell (Lawrence Livermore National Laboratory)

**Abstract :** A crucial concept for algebraic multigrid (AMG) coarsening and interpolation is that of strength of connection (SoC) between degrees of freedom. The classical SoC measure is based on the relative sizes of entries in each row of the matrix and relies on heuristics that assume an M-matrix structure. This simple measure is cheap to evaluate and successful for many problems, but also relies on a user-defined strength threshold, which may need to be tuned for specific problems. In addition, the classical SoC measure can have difficulty identifying the proper strong connections for operators that are not M-matrices, particularly when there are both positive and negative off-diagonal entries in the same row. In this work, we examine low-cost techniques for building an auxiliary strength matrix that shares important properties with the original matrix operator while also being more amenable to the classical SoC measure. Applying classical SoC to this auxiliary strength matrix improves robustness of the SoC measure for a wider class of problems and across a wider range of strength thresholds.

## [05263] Monolithic Multigrid and Block Preconditioning for Magnetic Confinement Fusion Relevant Resistive MHD Simulations

**Format :** Talk at Waseda University

**Author(s) :** Peter Ohm (RIKEN Center for Computational Science)John Shadid (Sandia National Laboratories)Jesus Bonilla (Los Alamos National Lab)Edward Phillips (Sandia National Laboratories)Raymond Tuminaro (Sandia National Laboratories)Jonathan Hu (Sandia National Laboratories)Xian-Zhu Tang (Los Alamos National Lab)Michael Crockatt (Sandia National Laboratories)

**Abstract :** A base-level mathematical basis for the continuum fluid modeling of dissipative plasma system is the resistive magnetohydrodynamic model. This model requires the solution of the governing partial differential equations (PDEs) describing conservation of mass, momentum, and thermal energy, along with various reduced forms of Maxwell's equations for the electromagnetic fields. The resulting systems are characterized by strong nonlinear and nonsymmetric coupling of fluid and electromagnetic phenomena, as well as the significant range of time- and length-scales that these interactions produce. These characteristics make scalable and efficient iterative solution, of the resulting poorly-conditioned discrete systems, extremely difficult.

In this talk we utilize Drekar, a multi-physics simulation code built on top of the Trilinos framework, for the simulation of various resistive MHD problems. We consider the use of block preconditioners as well as monolithic multigrid for solving coupled physics block systems.

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01170 (3/3) : 5D @E708 [Chair: Graham Harper]

## [03865] Combined On/Off Node Performance Model for SPMV in Multigrid

**Format :** Talk at Waseda University

**Author(s) :** Chris Siefert (Sandia National Laboratories)

**Abstract :** We propose combining traditional on-node memory-bandwidth based performance models (i.e., roofline) with inter-node performance models (i.e., ping-pong) to build a combined performance model to predict the performance of sparse matrix-vector products in the context of the Trilinos/MueLu algebraic multigrid software. We demonstrate the combined model on both CPU and GPU platforms and compare against actual Trilinos sparse matrix-vector product (SPMV) performance using Trilinos/MueLu.

## [05232] Recent Advances in Linear Solvers for Ice Sheet Modeling

**Format :** Talk at Waseda University

**Author(s) :** Jonathan Hu (Sandia National Laboratories)Jerry Watkins (Sandia National Laboratories)Max Carlson (Sandia National Laboratories)Mauro Perego (Sandia National Laboratories)Kim Liegeois (Sandia National Laboratories)Oscar Antepara (Lawrence Berkeley National Laboratory)Samuel Williams (Lawrence Berkeley National Laboratories)

**Abstract :** We present recent ongoing work performed under the SciDAC FAnSSIE project to improve linear solver performance within land-ice simulations on GPU-based architectures. We'll review the current algorithmic approach that relies on specialized semicoarsening algebraic multigrid, challenges in adapting this approach to GPU architectures, and progress in improving performance and scaling. Finally, we'll present numerical results from the Albany simulation code on the HPE Cray Ex supercomputer Perlmutter.

## [05118] A Matrix-Free Approach for Algebraic Multigrid for High-Order Systems

**Format :** Talk at Waseda University

**Author(s) :** Graham Harper (Sandia National Laboratories)

**Abstract :** We present a matrix-free approach for algebraic multigrid (AMG) for high-order systems. In particular, we focus on the case where an application may have a mix of domains with geometric structure and regions without geometric structure. We mix geometric multigrid (GMG) and AMG, but we approach the overall problem from a matrix-free AMG perspective on the finer levels. We present numerical results using Trilinos and MueLu to verify our methods.

## [03319] Mixed formulations and monolithic multigrid methods for smectic-A liquid crystals

**Format :** Online Talk on Zoom

**Author(s) :** Abdalaziz Hamdan (Imperial College London)Patrick Farrell (University of Oxford)Scott MacLachlan (Memorial University of Newfoundland)

**Abstract :** Xia et al. recently proposed a new continuum model for smectic A liquid crystals. Here, we present a mixed finite-element formulation of that model and discuss the construction of solvers for the resulting nonlinear systems. We consider Newton-Krylov-Multigrid approaches, using Newton's method to linearize and develop monolithic geometric multigrid preconditioners for the resulting saddle-point systems. We demonstrate this is an effective solver strategy when using a coupled "star" relaxation scheme and nested iteration.

## [01174] Hypernetworks and their dynamics in theory and applications

**Session Time & Room :** 5D (Aug.25, 15:30-17:10) @G704

**Type :** Proposal of Minisymposium

**Abstract :** Collective dynamics of interacting units are prevalent in nature and engineering, whether it is neurons in the brain or opinion building in social networks. Recently, there has been tremendous interest in simultaneous interactions between three or more units, so-called higher-order interactions. The drive comes from various disciplines, for example ecology, where simultaneous competition for resources of multiple species causes nonstationary fluctuations of species abundances. Such advances suggest to model the underlying structures by hypernetworks represented by hypergraphs.

This minisymposium displays recent models in real-world applications and theoretical studies on hypernetwork dynamics to highlight development and connect experts from both communities.

**Organizer(s) :** Christian Bick, Sören von der Gracht

**Classification :** 37C20, 93A16, 05C65, 92D25, 92D30, Network dynamics

**Minisymposium Program :**

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01174 (1/1) : 5D @G704 [Chair: Sören von der Gracht]

## [04246] Bridging between higher-order mechanisms and phenomena

**Format :** Talk at Waseda University

**Author(s) :** Giovanni Petri (CENTAI)

**Abstract :** Complex networks have become the main paradigm for modelling the dynamics of complex interacting systems.

However, networks are intrinsically limited to describing pairwise interactions, whereas real-world systems are often characterized by higher-order interactions involving groups of three or more units.

Higher-order structures, such as hypergraphs and simplicial complexes, are therefore a better tool to map the multilayered real organization of many social, biological and man-made systems. At the same time, higher-order observables, typically topological or information-theoretic in nature and often sharing the same simplicial language, have been gathering attention for their capacity to capture properties of complex systems that are invisible to standard statistical descriptions. This had led to a certain confusion between these two facets, mechanisms on one side, phenomena on the other.

Here, using recent examples from both dynamical models and neuroimaging analysis, I highlight collective behaviours induced by higher-order interactions, the difficulty in linking data and models through recent advances in topological data analysis and higher-order information theory, and finally outline key open questions for the physics of higher-order complex systems.

## [03667] Emergent hypernetworks in weakly coupled oscillators

**Format :** Talk at Waseda University

**Author(s) :** Eddie Nijholt (Imperial College London)Jorge Luis Ocampo-Espindola (Saint Louis University)Deniz Eroglu (Kadir Has University)István Kiss (Saint Louis University)Tiago Pereira (Universidade de São Paulo)

**Abstract :** Networks of weakly coupled oscillators play a profound role in our understanding of complex systems.

Studies on model reconstruction from data show the emergence of hyper-connections corresponding to triplet and higher-order interactions among oscillators, even though such models were originally defined as networks with only pairwise interactions. We show that hypernetworks can spontaneously appear in the presence of pairwise, albeit nonlinear, coupling given certain frequency resonance conditions. The conceptual explanation is that model reconstruction finds the so-called normal form of the system instead, which allows us to predict the emergent hypernetwork in terms of appearing and forbidden motifs. These results are moreover demonstrated in experiments with electrochemical oscillators. This is joint work with Jorge Luis Ocampo-Espindola, Deniz Eroglu, István Z. Kiss and Tiago Pereira.

## [04161] Do higher-order interactions promote coexistence in diverse ecological communities?

**Format :** Talk at Waseda University

**Author(s) :** Theo L Gibbs (Princeton University)Gabriel Gellner (University of Guelph)Simon Levin (Princeton University)Kevin McCann (University of Guelph)Alan Hastings (UC Davis)Jonathan Levine (Princeton University)

**Abstract :** Most ecological models assume that species interactions operate only between pairs of species. In a diverse community, however, higher-order interactions can emerge, in which two or more species jointly impact the growth of a focal species. In this talk, I will discuss two ways that higher-order interactions affect species coexistence. Randomly-sampled higher-order interactions do not promote coexistence, but additional constraints on the higher-order interactions can reverse exclusions caused by pairwise interactions.

## [04389] Hypernetworks: cluster synchronization is a higher order effect

**Format :** Talk at Waseda University

**Author(s) :** Bob Rink (Vrije Universiteit Amsterdam)Eddie Nijholt (Imperial College London)Sören von der Gracht (Paderborn University)

**Abstract :** Many networked systems are governed by non-pairwise interactions that can be encoded by means of a hypernetwork. Here, we define dynamical systems on hypernetworks, and we explain how to classify robust cluster synchronization patterns by finding balanced partitions. We show that synchronization is determined by polynomial systems of high order. Hence, unlike in dyadic networks, cluster synchronization on hypernetworks is a higher-order, nonlinear effect. We show how this generates remarkable synchrony breaking bifurcations.

## [01178] On the Interplay between Kinetic Theory and Quantum Dynamics

**Session Time & Room :**

01178 (1/2) : 2C (Aug.22, 13:20-15:00) @G802

01178 (2/2) : 2D (Aug.22, 15:30-17:10) @G802

**Type :** Proposal of Minisymposium

**Abstract :** The kinetic theory describes the non-equilibrium dynamics of a many-body system from the statistical viewpoint, which is acknowledged to be a significant model to bridge the microscopic and macroscopic regimes in classical mechanics. On the other hand, many novel quantum phenomena emerge in the physics and material fields, where the microscopic description is the quantum many-body system.

Hence, applying the kinetic philosophy to study the many-body systems in the quantum field becomes pretty natural, and this Minisymposium aims at fostering the development of multiscale modeling, mathematical analysis, and numerical simulation about the interplay between kinetic theory and quantum dynamics.

**Organizer(s) :** Kunlun Qi, Li Wang

**Classification :** 35Qxx, 81Qxx, 81Vxx, 82Cxx

**Minisymposium Program :**

01178 (1/2) : 2C @G802 [Chair: Kunlun Qi]

## [04305] Emergent phenomena in an interacting Bose gas

**Format :** Online Talk on Zoom

**Author(s) :** Michael Hott (University of Minnesota)Thomas Chen (The University of Texas at Austin)

**Abstract :** The study of kinetic equations describing collisions between a BEC and the surrounding normal fluid go back to Kirkpatrick and Dorfmann '83, '85 and Eckern '84. Ever since, this subject has attracted a lot of attention as it relates to condensation. In this context, mathematicians have studied the quartic quantum Boltzmann equation in the presence of a BEC. In this talk, we will discuss some of the progress made on the PDE level of the quantum Boltzmann equation. Then, we will focus on the validity of the kinetic equations. We will describe the crucial scale separations needed to extract a Boltzmann equation from the quantum dynamics. Moreover, we will see how the interference of sound waves can produce some surprising effects if a Bose gas is trapped in a volume of unit size. This is based on joint work with Thomas Chen.

## [05382] Fluid limits from Quantum Boltzmann equation

**Format :** Talk at Waseda University

**Author(s) :** Ning Jiang (Wuhan University)

**Abstract :** In his 2015 Ecole Polytechnique thesis, T.Zakrevskiy formally derived some fluid dynamics from quantum Boltzmann equation (Fermi-Dirac statistics). We rigorously justify two types of limits: incompressible Navier-Stokes-Fourier and compressible Euler (then acoustic) systems, by establishing some new nonlinear estimates on triple terms, and uniform estimates with respect to Kundsen number. A particular novelty is that the compressible Euler system derived from the quantum Boltzmann equation has a pressure law which is different and more general with that from the classical Boltzmann equation.

## [04436] An explicit coercivity estimate of the linearized quantum Boltzmann operator

**Format :** Talk at Waseda University

**Author(s) :** YULONG ZHOU (Sun Yat-Sen University)

**Abstract :** The Boltzmann-Bose-Einstein equation describes a large system of Bose-Einstein particles in the weak-coupling regime. If the particle interaction is governed by the inverse power law, the corresponding collision kernel has angular singularity. We present a coercivity estimate of the linearized Boltzmann-Bose-Einstein operator for such kernel. The estimate may not be sharp but explicitly reveals the dependence on the fugacity parameter. Joint work with Prof. Tong Yang.

## [04331] Frozen Gaussian Approximation for open quantum system

**Format :** Talk at Waseda University

**Author(s) :** Geshuo Wang (National University of Singapore)Zhenning Cai (National University of Singapore)Siyao Yang (National University of Singapore)

**Abstract :** We study the system-bath dynamics for open quantum systems applying frozen Gaussian approximation, which proposes an approximated ansatz for the wave function, converting the direct calculation of the Schrödinger equation into some ODEs of the parameters in the ansatz. We then derive the Dyson series under such approximation. To further improve the computational efficiency, we develop a fast algorithm known as the inchworm algorithm for the current framework.

01178 (2/2) : 2D @G802 [Chair: Ning Jiang]

## [04798] Quantum Dynamics of Incommensurate System

**Format :** Talk at Waseda University

**Author(s) :** Diyi Liu (University of Minnesota, Twin Cities)

**Abstract :** Motivated by the need to develop accurate numerical methods for computing the electronic properties of twisted bilayer graphene, we consider the problem of numerically computing the dynamics of a general aperiodic discrete (tight-binding) Schrödinger equation in an infinite domain. We prove that, under appropriate conditions, these dynamics can be rigorously approximated by those of a finite-dimensional truncated model. The key role in the proof is played by speed of propagation estimates derived from Combes-Thomas estimates. Besides the general aperiodic medium, we further improve our truncation analysis and Combes-Thomas Estimate for aperiodic medium with low dimensional structure, general van der Waal heterostructures. We then present a range of numerical experiments showing the effectiveness of our analysis.

## [04339] On the kinetic description of the objective molecular dynamics

**Format :** Talk at Waseda University

**Author(s) :** Kunlun Qi (University of Minnesota) Li Wang (University of Minnesota)

**Abstract :** In this talk, we will introduce a multiscale hierarchy framework for objective molecular dynamics (OMD), a reduced molecular dynamics with certain symmetry, that connects it to the statistical kinetic equation, and the macroscopic hydrodynamic model. In the mesoscopic regime, we exploit two interaction scalings that lead to either a mean-field type or a Boltzmann-type equation. At the macroscopic level, we also derive the corresponding reduced Euler and Navier-Stokes systems by conducting a detailed asymptotic analysis.

## [01181] Variational methods for multi-scale dynamics

**Session Time & Room :**

01181 (1/2) : 4C (Aug.24, 13:20-15:00) @F401

01181 (2/2) : 4D (Aug.24, 15:30-17:10) @F401

**Type :** Proposal of Minisymposium

**Abstract :** Many interesting evolutionary problems in nature can be described by variational principles like gradient flows or Hamiltonian dynamics. Recent results have shown that exploiting the variational structure of the evolution equation provides a fruitful research area combining applied analysis and stochastic modeling. For real-world multi-scale problems, focusing on the variational structure is particularly vital as it forms a physically motivated basis.

The aim of this two-part minisymposium is inspiring and bringing together researchers interested in calculus of variations, PDEs and stochastic analysis for starting collaborations. Focus is placed on interacting particle systems and discrete-to-continuous limit passages, e.g. by evolutionary Gamma-convergence.

**Organizer(s) :** Yuan Gao, Matthias Liero, Artur Stephan

**Classification :** 49Jxx, 35-xx, 70-xx, 60Jxx, 82Cxx

**Minisymposium Program :**

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01181 (1/2) : 4C @F401 [Chair: Artur Stephan]

## [04903] Controlling conservation laws: Entropy-Entropy flux pairs

**Format :** Talk at Waseda University

**Author(s) :** Wuchen Li (University of South Carolina)

**Abstract :** In this talk, we study a class of variational problems for regularized conservation laws with Lax's entropy-entropy flux pairs. We first introduce a modified optimal transport space based on conservation laws with diffusion. Using this space, we demonstrate that conservation laws with diffusion are "flux-gradient flows." We next construct variational problems for these flows, for which we derive dual PDE systems for regularized conservation laws. Several examples, including traffic flow and Burgers' equation, are presented. We successfully compute the control of conservation laws by incorporating both primal-dual algorithms and monotone schemes. This is based on joint work with Siting Liu and Stanley Osher.

## [03821] Transport problems with non linear mobilities: a particle approximation result.

**Format :** Talk at Waseda University

**Author(s) :** Lorenzo Portinale (Hausdorff Center for Mathematics, Bonn) Simone Di Marino ( Università di Genova ) Emanuela Radici ( Università degli Studi dell'Aquila)

**Abstract :** We study discretisation of generalised Wasserstein distances with non linear mobilities on the real line via a Riemannian metrics on the space of N ordered particles. In particular, we provide a  $\Gamma$ -convergence result for the associated discrete metrics as  $N \rightarrow \infty$  to the continuous one and discuss applications to the approximation of one-dimensional conservation laws (of gradient flow type) via the so-called generalised minimising movements (or JKO scheme).

## [04444] Variational convergence for irreversible population dynamics

**Format :** Talk at Waseda University

**Author(s) :** Jasper Hoeksema (Eindhoven University of Technology)

**Abstract :** We consider the forward Kolmogorov equations corresponding to measure-valued processes stemming from a class of interacting particle systems in population dynamics. In contrast to previous work, where we assumed detailed balance, we will now treat the irreversible case. We exchange gradient structures for more general dissipation structures, and show convergence of these structures in the large population limit. In particular we obtain convergence to the mean-field limit and establish entropic propagation of chaos.

## [03883] Mathematical modeling of structured magnesium alloys

**Format :** Talk at Waseda University

**Author(s) :** Karel Svalenka (Kyoto University)

**Abstract :** Structured materials, such as metallic alloys with atomic-scale layers, show peculiar deformation patterns, which may have significant implications on material properties. In this talk, I will discuss one possible approach to modeling of this kind of pattern formation through the so-called rate-independent evolution in the variational setting of finite-strain elasto-plasticity. Besides mentioning connections to homogenization via Gamma-convergence, I will present the underlying mathematical theory and show numerical simulations in comparison to experimental measurements.

01181 (2/2) : 4D @F401 [Chair: Jasper Hoeksema]

## [04828] Variational numerical schemes for gradient flows

**Format :** Online Talk on Zoom

**Author(s) :** Yiwei Wang (University of California, Riverside)Chun Liu (Illinois Institute of Technology)

**Abstract :** We'll present a numerical framework for developing structure-preserving variational schemes for various types of gradient flows. The numerical approach starts with the energy-dissipation law of the underlying system and can combine different spatial discretizations, including Eulerian, Lagrangian, particle, and neural-network-based approaches. The numerical procedure guarantees the developed schemes are energy stable and can preserve the intrinsic physical constraints. Several applications and theoretical justifications will be discussed.

## [04971] Quantitative coarse-graining of Markov chains

**Format :** Online Talk on Zoom

**Author(s) :** Upanshu Sharma (UNSW Sydney)Bastian Hilder (Lund University)

**Abstract :** Coarse-graining is the procedure of approximating large and complex systems by simpler and lower-dimensional ones. It is typically characterised by a mapping which projects the full state of the system onto a smaller set; this mapping captures the relevant (often slow) features of the system. Starting from a (non-reversible) continuous-time Markov chain and such a mapping, I will discuss an effective dynamics which approximates the true projected Markov chain and present error estimates on the approximation error.

## [04391] Variational convergence from mean-field stochastic particle systems to the exchange-driven growth model

**Format :** Online Talk on Zoom

**Author(s) :** Chun Yin Lam (Universität Münster)André Schlichting (Universität Münster)

**Abstract :** We consider the hydrodynamic limit of mean-field stochastic particle systems on a complete graph using variational methods.

The evolution is driven by particle exchanges with its rate depending on the population of the initial and final vertices. This model is a generalisation of the zero-range process and has applications in cloud formation, polymerization, and wealth exchange.

Under detailed balance conditions, the evolution equation has a gradient structure motivated by the Large Deviations Principle. The variational formulation is based on the LDP rate function.

## [05130] On time-splitting methods for gradient flows with two dissipation mechanisms

**Format :** Talk at Waseda University

**Author(s) :** Artur Stephan (Weierstrass Institute for Applied Analysis and Stochastics, Berlin, Germany)

**Abstract :** A gradient system consists of a state space  $X$ , an energy functional  $E : X \rightarrow \mathbb{R} \cup \{\infty\}$  and a dissipation potential  $R : X \rightarrow \mathbb{R}$  to

### [0, infinity[\$ and defines a gradient-flow equation.

Considering the case where the dual dissipation potential  $R^*$  is given by the sum  $R^* = R_1^* + R_2^*$ , we show how convergence of a time-splitting method where the solution of the combined gradient system is approximated by concatenating the separate gradient-flows.

This is joint work with Alexander Mielke (Berlin) and Riccarda Rossi (Brescia).

## [01188] Recent Developments in Fluid Dynamics

**Session Time & Room :**

01188 (1/3) : 2C (Aug.22, 13:20-15:00) @G405

01188 (2/3) : 2D (Aug.22, 15:30-17:10) @G405

01188 (3/3) : 2E (Aug.22, 17:40-19:20) @G405

**Type :** Proposal of Minisymposium

**Abstract :** Over the last years, substantial breakthroughs have arisen in mathematical fluid mechanics. For example, the smooth blowup of the incompressible, axisymmetric Euler equations via computer assisted proofs, or the smooth self-similar blowup solutions to compressible Euler and Navier-Stokes. The aim of this session is to bring together well-known experts and young researchers to present new developments in partial differential equations describing the dynamics of fluids. Particular emphasis has been put into explaining the aforementioned breakthroughs and exploring new directions from them. Other key topics include corners and cusps solutions in fluids models, and stability results for kinetic equations.

**Organizer(s) :** Bruno Vergara, Javier Gómez Serrano

**Classification :** 35-XX

**Minisymposium Program :**

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01188 (1/3) : 2C @G405 [Chair: Javier Gómez Serrano]

## [04609] Recent progress on singularity formation in incompressible fluids

**Format :** Online Talk on Zoom

**Author(s) :** Jiajie Chen (New York University) Thomas Y Hou (California Institute of Technology)

**Abstract :** I will talk about recent progress on singularity formation in incompressible fluids with smooth data.

## [04708] Gravity Unstable Muskat Bubbles

**Format :** Online Talk on Zoom

**Author(s) :** Neel Patel (University of Maine) Siddhant Agrawal (ICMAT) Sijue Wu (University of Michigan)

**Abstract :** The Muskat problem describes the evolution of the interface between two fluids in porous media. Neglecting surface tension, the well-posedness of this problem depends on the Rayleigh-Taylor condition. For fluids of differing densities, it is required that the denser fluid is below. Otherwise, the system is gravity unstable. We will discuss the stability of a closed curve interface, or a bubble, in which the Rayleigh-Taylor condition cannot hold.

## [04950] Whitham's highest cusped wave

**Format :** Talk at Waseda University

**Author(s) :** Bruno Vergara (Brown University)

**Abstract :** Whitham's equation is a nonlinear, nonlocal, very weakly dispersive shallow water wave model in one space dimension. As in the case of the Stokes wave for the Euler equation, non-smooth traveling waves with greatest height between crest and trough have been shown to exist for this model. In this talk I will discuss the existence of a unique cusped, convex and monotone traveling wave solution to the Whitham equation. Our results follow a strategy that combines different ideas from classical analysis and rigorous computer verification methods. Joint work with Alberto Enciso and Javier Gómez Serrano.

## [03258] On the (in)stability of smooth self-similar solutions to the compressible Euler equations

**Format :** Talk at Waseda University

**Author(s) :** Anxo Farina Biasi (Ecole Normale Supérieure-Paris)

**Abstract :** In this talk, I am going to describe recent progress in smooth self-similar solutions to the compressible Euler equations. I will explain how these solutions, initially found by Merle-Raphael-Rodnianski-Szeftel (2019), arise in the family of Guderley self-similar solutions (1942), how their (in)stability is studied under smooth perturbations, and which are some endpoints of unstable directions. The topic will be introduced making a contrast between its states during the 20th and 21st centuries.

01188 (2/3) : 2D @G405 [Chair: Bruno Vergara]

## [04242] Small scale creation for the 2D Boussinesq Equation

**Format :** Talk at Waseda University

**Author(s) :** Alexander Kiselev (Duke University) Yao Yao (National University of Singapore) Jaemin Park (University of Basel)

**Abstract :** In this talk, we study long-time behaviors of the two-dimensional incompressible Boussinesq equations without thermal diffusion. While the 2D Boussinesq equations are known to possess global solutions with the presence of viscosity, it remains an outstanding open problem whether the inviscid case can exhibit a finite-time blow up. In the viscous case, we established algebraic growth of the Sobolev norms of the solutions for all time. For the inviscid case, we obtained the growth of the gradient of the temperature, assuming that the global solution exists for all time. The initial data under consideration in this work is not too restrictive. More precisely, we only require certain symmetry and sign conditions. The key ingredient of the proof is to derive a norm-inflation from the decay of an anisotropic Sobolev norm of the temperature, which can be observed in the conservation of energy. This work is a joint work with A. Kiselev and Y. Yao.

## [05046] On the motion of an internal wave in two-dimensional viscous flow

**Format :** Talk at Waseda University

**Author(s) :** Rafael Granero-Belinchon (Universidad de Cantabria)

**Abstract :** In this talk we will review some recent results concerning the motion of an internal wave in two-phase viscous flow. In particular we will establish the local and global well-posedness of the free boundary problem associated to this physical situation. Finally, we will also prove an exponential instability result.

These results were obtained in a joint work with Francisco Gancedo and Elena Salguero.

## [03025] Smooth imploding solutions for 3D compressible fluids

**Format :** Online Talk on Zoom

**Author(s) :** Gonzalo Cao Labora (Massachusetts Institute of Technology (MIT))

**Abstract :** We will talk about singularity formation for the 3D isentropic compressible Euler and Navier-Stokes equations for ideal gases. We will construct a new family of self-similar profiles corresponding to larger self-similar exponents than what was previously known. In particular, this will show singularity formation for all adiabatic

constants, giving the first known singularity formation result for monoatomic gases. These results are joint work with Tristan Buckmaster and Javier Gomez-Serrano.

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01188 (3/3) : 2E @G405 [Chair: Bruno Vergara]

### [04870] Stability of a point charge for the Vlasov-Poisson system

**Format :** Online Talk on Zoom

**Author(s) :** Benoit Pausader (Brown University)

**Abstract :** We consider solutions of the Vlasov-Poisson system starting from initial data (i) a dirac mass (the point charge) and (ii) some small density with respect to Liouville measure (the cloud). We show global existence of the solution and describe the asymptotic behavior in terms of modified scattering. This is joint work with K. Widmayer and J. Jiang.

### [05033] Global axisymmetric Euler flows with rotation

**Format :** Online Talk on Zoom

**Author(s) :** Klaus Widmayer (University of Vienna & University of Zurich)Benoit Pausader (Brown University)Yan Guo (Brown University)

**Abstract :** We discuss the construction of a class of global, dynamical solutions to the 3d Euler equations near the stationary state given by uniform "rigid body" rotation. These solutions are axisymmetric, of Sobolev regularity and have non-vanishing swirl.

### [02875] On the analyticity of the Muskat equation

**Format :** Online Talk on Zoom

**Author(s) :** Jia Shi (MIT)

**Abstract :** The Muskat equation describes the interface of two liquids in a porous medium. We will show that if a solution to the Muskat problem in the case of same viscosity and different densities is sufficiently smooth, then it must be analytic except at the points where a turnover of the fluids happens. We will also show analyticity in a region that degenerates at the turnover points provided some additional conditions are satisfied.

## [01190] Recent Advances in Modeling Complex Systems and Multiscale Problems in Mathematical Biology

**Session Time & Room :**

01190 (1/2) : 5C (Aug.25, 13:20-15:00) @E802

01190 (2/2) : 5D (Aug.25, 15:30-17:10) @E802

**Type :** Proposal of Minisymposium

**Abstract :** Advances in our understanding of complex problems in biology are aided by mathematical modeling. A common challenge in this effort is incorporating a wide range of temporal and spatial scales into a single model. This symposium will explore a variety of biological systems, such as microtubule polymerization and blood coagulation, and the diversity of methods used to examine them, such as dynamical systems theory and numerical methods. Our proposed speakers from the US and Canada represent various stages in academia and highlight the versatility of modeling as a tool to answer active biological questions.

**Organizer(s) :** Anna Nelson, Keshav Patel

**Classification :** 92C30, 92C05, 92C37, 92C35

**Minisymposium Program :**

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01190 (1/2) : 5C @E802 [Chair: Keshav Patel]

## [04951] A Spatially Averaged Model for Platelet Cohesion by vWF

**Format :** Talk at Waseda University

**Author(s) :** Keshav Bhavesh Patel (University of Utah)Aaron Fogelson (University of Utah)

**Abstract :** Platelet aggregation in high shear rate environments, in both healthy and stenotic arterioles, is mediated by Von Willebrand Factor (vWF). Computational fluid dynamics (CFD) models can study this process but are time-intensive and unable to explore sets of physiologically relevant parameters. In this talk, we will discuss a spatially averaged dynamical systems model of platelet aggregation. We quantify how vWF reduces aggregation time at high shear rates and determine essential parameters involved in aggregate formation.

## [04400] Investigating traveling waves in biophysical models of cardiac dynamics

**Format :** Talk at Waseda University

**Author(s) :** Stephanie Dodson (Colby College)Timothy Lewis (University of California Davis)

**Abstract :** Regular cardiac function is characterized by coherent traveling waves of electrical activity that drive heart beats. When this process goes awry, the ensuing irregular rhythms are known as arrhythmias, which can be life-threatening. Hence, it is crucial to understand conditions that influence arrhythmia onset. In previous work, these traveling waves have been mathematically investigated in qualitative models of excitable media. We investigate traveling wave properties and arrhythmia onset using biophysically realistic models of cardiac dynamics.

## [05165] Modeling and Simulation of Mucin-like Polyelectrolyte Gels

**Format :** Talk at Waseda University

**Author(s) :** Owen Lewis (University of New Mexico)Jian Du (Florida Institute of Technology)Aaron L Fogelson (University of Utah)James P Keener (University of Utah)

**Abstract :** Volume phase transitions in polyelectrolyte gels play important roles in many biophysical processes such as mucus secretion, DNA packaging, nerve excitation, and cellular secretion. The swelling and deswelling of these charged polymer gels depend strongly on their ionic environment. In this paper, we present an extension to our previous two-fluid model for ion-binding-mediated gel swelling. The model treats the polyelectrolyte gel as a mixture of two continuum materials, the network and the solvent. We use mean-field arguments to derive the force densities that nano-scale species (ions and individual solvent particles) exert on these two species. The resulting model is suitable for the investigation of a large family of biologically relevant problems.

## [04304] Adaptive IMEX method for fractional PDE in viscoelastic fluids

**Format :** Talk at Waseda University

**Author(s) :** Dipa Ghosh (IIIT DELHI)

**Abstract :** Fractional PDEs have emerged as a powerful tool for modelling multiphysics and multiscale processes in numerical simulations ranging from physics and biology to quantitative finance. We propose a novel family of time-asymptotically stable, implicit-explicit, adaptive time integration methods for the solution of the fractional advection-diffusion-reaction equations. The fractional diffusion equation (2D) and the incompressible, subdiffusive dynamics of the Rouse chain melts ( $\alpha = 1/2$ ) and the Zimm chain solution ( $\alpha = 2/3$ ) are used to assess the method.

01190 (2/2) : 5D @E802 [Chair: Anna Nelson]

## [04322] A mathematical model of microtubule assembly and polarity in dendrites

**Format :** Talk at Waseda University

**Author(s) :** Anna Nelson (Duke University)Veronica Ciocanel (Duke University)Scott McKinley (Tulane University)

**Abstract :** The microtubule cytoskeleton is responsible for sustained transport of cellular cargo inside neurons. However, microtubules must also be dynamic and rearrange their orientation in response to injuries. We introduce a spatially-explicit mathematical model of dendritic microtubule growth dynamics using parameters informed by experimental data. We explore several hypotheses of microtubule growth using both a stochastic model and a continuum model, and use fluorescence microscopy experiments to validate mechanisms such as limited tubulin and length-dependent catastrophe.

## [04441] Parameter Estimation for Mechanistic Models of Tear Film Breakup

**Format :** Talk at Waseda University

**Author(s) :** Rayanne A Luke (George Mason University)Richard J Braun (University of Delaware)Tobin A Driscoll (University of Delaware)Deborah Awisi-Gyau (Alcon Research LLC)Carolyn G Begley (Indiana University)

**Abstract :** Tear film breakup is related to dry eye disease. Breakup causes include evaporation and divergent flow; related quantities cannot be directly measured during breakup. We determine such variables by fitting thin film fluid dynamics models for breakup to experimental data. Our results suggest that evaporation and divergent flow cooperate to drive faster breakup; purely evaporative cases exhibit slower thinning. These results are the first to make a tight comparison between such models and experimental data.

## [05183] Modelling Glucose Regulation: Lipotoxicity and the Progression to Type 2 Diabetes

**Format :** Talk at Waseda University

**Author(s) :** Katharine R Faulkner (University of British Columbia)

**Abstract :** As an individual moves from healthy to pre-diabetic to diabetic, there are many physiological changes that occur, but it is not known which of these changes are the main drivers of the progression to type II diabetes. In this talk, I will describe a simple model for glucose regulation and how modeling can help determine which of these physiological changes are capable of pushing an individual from healthy to diseased. By framing this problem in terms of bifurcations, we can find models that create qualitative changes to the system that allow for movement between healthy and diseased states. We will examine a model that includes the toxicity of lipids in the pancreas, and find a bifurcation that describes the progression to type II diabetes.

## [04351] PIEZO1 regulates cellular coordination during collective cell migration

**Format :** Talk at Waseda University

**Author(s) :** Jinghao Chen (University of California, Irvine)Jesse Holt (University of California, Irvine)Beth Evans (University of California, Irvine)John Lowengrub (University of California, Irvine)Medha Pathak (University of California, Irvine)

**Abstract :** The mechanically-activated ion channel PIEZO1 was recently identified to play an inhibitory role during wound healing. Through an integrative experimental and mathematical modeling approach, we elucidate PIEZO1's contributions to keratinocyte collective migration, an essential component of the healing process. Here, through a 2D-multiscale model of wound closure which links observations at both the single and multicell scales, and subsequent experimental validation, we identify cell directionality as being impacted by PIEZO1 activity during wound closure.

## [01191] Recent advances on regularity and irregularity of fluids flows

**Session Time & Room :**

01191 (1/3) : 1C (Aug.21, 13:20-15:00) @G703

01191 (2/3) : 1D (Aug.21, 15:30-17:10) @G703

01191 (3/3) : 1E (Aug.21, 17:40-19:20) @G703

**Type :** Proposal of Minisymposium

**Abstract :** Building a satisfactory mathematical theory of turbulence remains one of the most significant challenges in the physical sciences, with several fundamental problems still open. Deeply tied to these problems are issues associated with the regularity and well-posedness of fluid flows. Recent developments have shed light on the chaotic behavior of turbulent flows, the role of criticality in ill-posedness, singularity formation in classical solutions, and the relation between irregularity, instability, and non-uniqueness of solutions. The goal of this session is to gather those who have contributed to these developments, promote the exchange of ideas, and inspire new ones.

**Organizer(s) :** Aseel Farhat, Evelyn Lunasin, Vincent Martinez

part\_2

**Classification :** 35Q30, 35Q35, 35B65, 76F20, 37N10**Minisymposium Program :**

01191 (1/3) : 1C @G703 [Chair: Evelyn Lunasin]

**[03313] Singularity formation for models of fluids****Format :** Talk at Waseda University**Author(s) :** Mimi Dai (University of Illinois at Chicago)**Abstract :** Finite time singularity formation for fluid equations will be discussed. Built on extensive study of approximating models, breakthroughs on this topic have emerged recently for Euler equation. Inspired by the progress for pure fluids, we attempt to understand this challenging issue for magnetohydrodynamics (MHD). Finite time singularity scenarios are discovered for some reduced models of MHD. The investigation also reveals connections of MHD with Euler equation and surface quasi-geostrophic equation.**[03731] Vorticity estimates for the 3D incompressible Navier-Stokes equation****Format :** Online Talk on Zoom**Author(s) :** Jincheng Yang (University of Chicago)**Abstract :** We show some a priori regularity estimates for the vorticity and its trace in the three-dimensional incompressible Navier-Stokes equation. These a priori estimates are obtained via the blow-up method and a novel averaging operator. The averaging operator can be used to provide regularity and trace estimates for PDEs with  $\varepsilon$ -regularity.**[04943] On criticality of the Navier-Stokes diffusion****Format :** Online Talk on Zoom**Author(s) :** zoran grujic (university of virginia)**Abstract :** The main purpose of this talk is to present a mathematical evidence of criticality of the Navier-Stokes diffusion. In particular, considering a plausible candidate for a finite time blow-up, a two-parameter family of the dynamically rescaled profiles, we show that as soon as the hyper-diffusion exponent is greater than one, a new region in the parameter space (completely in the super-critical regime) is ruled out. As a matter of fact, the region is a neighborhood (in the parameter space) of the self-similar profile, i.e., the 'approximately self-similar' blow-up is ruled out for all hyper-diffusive models.**[05062] Well-posedness of mildly regularized active scalars in Sobolev spaces****Format :** Online Talk on Zoom**Author(s) :** Anuj Kumar (Florida State University)Vincent Ryan Martinez (CUNY Hunter College)**Abstract :** In this work, we consider the initial value problem for a family of active scalar equations when perturbed by a logarithmic order regularization in dissipation. These equations, commonly known as generalized surface quasi-geostrophic equations (gSQG) interpolate between the 2D incompressible Euler equation and the 2D SQG equation, and extrapolate beyond SQG to a family with more singular velocities. Ill-posedness at the threshold regularity for the

unperturbed models has been established in the celebrated works of Bourgain and Li, and Elgindi and Masmoudi for the 2D Euler equation, and recently by Cordoba and Zoroa-Martinez, and Jeong and Kim for the 2D SQG equation. In this work, we treat the positive side of well-posedness and consider a minimally dissipative regularization to recover local well-posedness (in the Hadamard sense) in the threshold Sobolev regularity. The proof is based on developing estimates for a suitably identified linear system that preserves the underlying commutator structure of the nonlinearity.

01191 (2/3) : 1D @G703 [Chair: Vincent Martinez]

## [04347] Bounded weak solutions to the 2D quasi-geostrophic equation

**Format :** Online Talk on Zoom

**Author(s) :** Elaine Cozzi (Oregon State University)

**Abstract :** We outline a proof of global existence of bounded weak solutions to the 2D quasi-geostrophic equation (SQG), building on a result of Marchand. Our proof utilizes a Littlewood-Paley version of a Serfati type of identity for SQG. This is joint work with David Ambrose and Jim Kelliher.

## [02935] On the support of anomalous dissipation measures

**Format :** Online Talk on Zoom

**Author(s) :** Theodore D. Drivas (Stony Brook University)

**Abstract :** By means of a unifying measure-theoretic approach, we establish lower bounds on the Hausdorff dimension of the space-time set which can support anomalous dissipation for weak solutions of fluid equations, both in the presence or absence of a physical boundary. Boundary dissipation, which can occur at both the time and the spatial boundary, is analyzed by suitably modifying the Duchon & Robert interior distributional approach. One implication of our results is that any bounded Euler solution (compressible or incompressible) arising as a zero-viscosity limit of Navier-Stokes solutions cannot have anomalous dissipation supported on a set of dimension smaller than that of the space. This is joint work with L. De Rosa and M. Inversi.

## [03059] Kinetic shock profiles for the Landau equation

**Format :** Talk at Waseda University

**Author(s) :** Dallas Albritton (UW-Madison)

**Abstract :** Compressible Euler solutions develop jump discontinuities known as shocks. However, physical shocks are not, strictly speaking, discontinuous. Rather, they exhibit an internal structure which, in certain regimes, can be represented by a smooth function, the shock profile. We demonstrate the existence of weak shock profiles to the kinetic Landau equation. Joint work with Matthew Novack (Purdue University) and Jacob Bedrossian (UCLA).

## [04056] On sharp-crested water waves and finite-time singularity formation

**Format :** Online Talk on Zoom

**Author(s) :** Nastasia Grubic (ICMAT, CSIC)

**Abstract :** We show that the 2d gravity water waves system is locally wellposed in weighted Sobolev spaces which allow for interfaces with corners. These singular points are not rigid; if the initial interface exhibits a corner, it remains a corner but generically its angle changes. Using a characterization of the asymptotic behavior of the fluid near a corner that follows from our a-priori energy estimates, we show the existence of initial data in these spaces for which the fluid becomes singular in finite time.

01191 (3/3) : 1E @G703 [Chair: Aseel Farhat]

## [04796] Turbulent solutions of fluid equations

**Format :** Talk at Waseda University

**Author(s) :** Alexey Cheskidov (University of Illinois at Chicago)

**Abstract :** In the past couple of decades, mathematical fluid dynamics has been highlighted by numerous constructions of solutions to fluid equations that exhibit pathological or wild behavior. These include the loss of the energy balance, non-uniqueness, singularity formation, and dissipation anomaly. Interesting from the mathematical point of view, providing counterexamples to various well-posedness results in supercritical spaces, such constructions are becoming more and more relevant from the physical point of view as well. Indeed, a fundamental physical property of turbulent flows is the existence of the energy cascade. Conjectured by Kolmogorov, it has been observed both experimentally and numerically, but had been difficult to produce analytically. In this talk I will overview new developments in discovering not only pathological mathematically, but also physically realistic solutions of fluid equations.

## [03868] A localized maximum principle and its application to the critical SQG on bounded domain

**Format :** Talk at Waseda University

**Author(s) :** Tsukasa Iwabuchi (Tohoku University)

**Abstract :** We discuss a spectral localization technique for the Dirichlet Laplacian on smooth bounded domain to deal with the fractional Laplacian of the derivative order one and commutator estimates in the framework of Besov spaces. It corresponds to a generalization of the analysis by the dyadic decomposition of the frequency through the Fourier transform in the Euclidean space. As an application, we show the existence of global solutions of the surface quasi-geostrophic equation with the critical dissipation for small initial data.

## [03232] Speeding up Langevin Dynamics by Mixing

**Format :** Talk at Waseda University

**Author(s) :** Yuanyuan Feng (East China Normal University)Gautam Iyer (Carnegie Mellon University)Alexei Novikov (Penn State University)Alexander Christie (Penn State University)

**Abstract :** We add a drift to the Langevin dynamics (without changing the stationary distribution) and obtain quantitative estimates on the mixing time. We show that an exponentially mixing drift can be rescaled to make the mixing time of the Langevin system arbitrarily small.

## [04760] On intermittent strong Onsager conjecture

**Format :** Online Talk on Zoom

**Author(s) :** Hyunju Kwon (ETH Zurich)

**Abstract :** Smooth solutions to the incompressible 3D Euler equations, which are spatially periodic, are known to conserve kinetic energy in every local region. Turbulent flows, however, exhibit anomalous dissipation of kinetic energy, indicating the existence of a weak solution to the Euler equations with dissipation of kinetic energy in some region, but no creation of energy everywhere in the domain. This motivates the strong Onsager conjecture, which combines the original Onsager conjecture with the local energy inequality. In this talk, I will discuss the flexibility side of the  $L^3$ -based strong Onsager conjecture, adapting to the intermittent nature of turbulence, and introduce a wavelet-based convex integration scheme. The talk is based on a joint work with Matt Novack and Vikram Giri.

# [01195] Hyperbolic one-dimensional systems in networks: mathematical modeling and numerical approximations

**Session Time & Room :**

01195 (1/2) : 2D (Aug.22, 15:30-17:10) @G601

01195 (2/2) : 2E (Aug.22, 17:40-19:20) @G601

**Type :** Proposal of Minisymposium

**Abstract :** Gas flow in pipes, open channel flows, water distribution, traffic flow and blood flow are some modelling applications very often represented as hyperbolic one-dimensional systems in networks. Key modelling ingredients for these systems are the correct definition of boundary conditions at terminal network points, proper coupling conditions among one-dimensional domains and the coupling of one-dimensional domains to zero-dimensional models. Further complexity may be added: parameters varying in space and time, flow regimes varying from sub- to supercritical, diffusive and dispersive terms, etc. All these aspects result in challenging situations for numerical methods designed to discretise this type of models.

**Organizer(s) :** Ernesto Pimentel-García, Lucas O. Müller

**Classification :** 35L02, 35L03, 65M08, 65M06

**Minisymposium Program :**

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01195 (1/2) : 2D @G601 [Chair: Lucas O. Müller]

## [02382] Control of advection-diffusion equations on networks and singular limits

**Format :** Talk at Waseda University

**Author(s) :** Nicola De Nitti (FAU Erlangen-Nürnberg )

**Abstract :** We consider advection-diffusion equations posed on a tree-shaped network with suitable transmission conditions at the junctions. We study the asymptotic behavior of the cost of the null-controllability as the diffusivity parameter vanishes: we show that it decays for a sufficiently large time and explodes for short times with an exponential rate.

## [02297] A second order model of traffic with organization marker

**Format :** Talk at Waseda University

**Author(s) :** Abraham Sylla (University of Milano-Bicocca)

**Abstract :** We present a toy model for self-organized road traffic taking into account the state of orderliness in drivers' behavior. The model is reminiscent of the wide family of generalized second-order models of road traffic. The orderliness marker is evolved along vehicles' trajectories and it influences the fundamental diagram of the traffic flow. The coupling we have in mind is nonlocal, leading to a kind of "weak decoupling" of the resulting  $2 \times 2$  system.

## [02293] Limiting flow in atrial-ventricular function

**Format :** Talk at Waseda University

**Author(s) :** Javier Murillo (I3A, University of Zaragoza,)Juan Mairal (I3A, University of Zaragoza,)Pilar García-Navarro (I3A, University of Zaragoza,)

**Abstract :** To date, no methodology is available for coupling 1D blood flow to models of the peripheral vasculature, valves, or heart when the flow regime is other than subsonic. When modeling complex fluid networks using 1D approaches, boundary conditions can be imposed using 0D models. An application case is the modeling of the human circulation using closed-loop models. These can be considered a tool to investigate short-term transient hemodynamic responses to postural changes in atrial-ventricular function.

01195 (2/2) : 2E @G601 [Chair: Ernesto Pimentel-García]

## [02299] The Junction Riemann Problems under transonic scenarios: application to veins.

**Format :** Talk at Waseda University

**Author(s) :** Juan Mairal (I3A - Universidad de Zaragoza)Javier Murillo (I3A, University of Zaragoza,)Pilar García-Navarro (I3A - Universidad de Zaragoza)

**Abstract :** Current 1D numerical methods for flow in junctions provide good results in most cases. In the 1D framework, the junction is a singular point. One of the shortcomings of existing methods is their inability to deal with transonic and supersonic flow at junctions in physiological flows. Existing methods that rely on coupling approaches for conservation of mass, energy or momentum and the characteristic equations for subsonic flow conditions are revisited here.

## [02244] Numerical and physical impact of coupling conditions for one dimensional blood flow models

**Format :** Talk at Waseda University

**Author(s) :** Lucas Omar Müller (University of Trento)

**Abstract :** One dimensional blood flow models consist of hyperbolic or hyperbolic-dominant systems of balance laws. This specific mathematical property plays a key role in the derivation of coupling and boundary conditions necessary to model blood flow in networks of vessels. In this talk we will derive coupling and boundary conditions for a general velocity profile and study their physical and numerical impact in simulations of the arterial and venous system across several spatial scales.

## [02355] High-order fully well-balanced numerical methods for one-dimensional blood flow in networks

**Format :** Talk at Waseda University

**Author(s) :** Ernesto Pimentel-García (University of Málaga)

**Abstract :** We are interested in the numerical study of one-dimensional blood flow model in networks with discontinuous mechanical and geometrical properties. We do an exhaustive investigation of all its stationary solutions and we propose high-order fully well-balanced numerical methods that are able to preserve all of them. These methods are able to deal with more than one discontinuous parameter and friction. Some numerical tests are shown to prove its well-balanced and high-order properties.

## [01197] Numerical linear algebra in convex and nonconvex optimization

**Session Time & Room :** 3D (Aug.23, 15:30-17:10) @F311

**Type :** Proposal of Minisymposium

**Abstract :** Convex optimization has been instrumental in significant progress across science and technology. Nonconvex optimization methods are an exciting area of active research driven by modern applications. The efficiency and effectiveness of most optimization algorithms hinge on the numerical linear algebra algorithms that they utilize. Furthermore, optimization applications have motivated fundamental advances in numerical linear algebra. This minisymposium aims to bring together experts in both optimization and numerical linear algebra to discuss new developments and leading challenges in both areas.

**Organizer(s) :** Alexander Strang, Ming Gu

**Classification :** 65K10, 65Fxx, 90C26

**Minisymposium Program :**

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01197 (1/1) : 3D @F311 [Chair: Alexander Strang]

## [01875] Nonconvex accelerated gradient descent without parameter tuning

**Format :** Talk at Waseda University

**Author(s) :** Naoki Marumo (University of Tokyo)Akiko Takeda (University of Tokyo)

**Abstract :** We propose a new first-order method for minimizing nonconvex functions with a Lipschitz continuous gradient and Hessian. The proposed algorithm is an accelerated gradient descent method with two restart mechanisms. It finds a solution where the gradient norm is less than  $\varepsilon$  in  $O(\varepsilon^{-7/4})$  function and gradient evaluations. Unlike existing algorithms with similar complexity bounds, our method requires no prior knowledge of problem-dependent parameters. Several numerical results illustrate that the proposed method is promising.

## [02180] Low Rank Tensor Decompositions and Approximations

**Format :** Online Talk on Zoom

**Author(s) :** Jiawang Nie (University of California, San Diego)Li Wang (University of Texas, Arlington)Zequn Zheng (University of California, San Diego)

**Abstract :** There exist linear relations among tensor entries of low rank tensors. These linear relations can be expressed by multi-linear polynomials, which are called generating polynomials. We use generating polynomials to compute tensor rank decompositions and low rank tensor approximations. We prove that this gives a quasi-optimal low rank tensor approximation if the given tensor is sufficiently close to a low rank one.

## [05344] Efficient and numerically stable interior-point algorithms for convex optimization

**Format :** Online Talk on Zoom

**Author(s) :** Ming Gu (UC Berkeley)

**Abstract :** We present efficient and numerically stable interior-point algorithms for linear programs, quadratic programs, as well as second order cone programs (socp), with supporting numerical results. In particular, our

part\_2

stable algorithms for socp  
 achieves full machine precision accuracy, whereas existing interior-point methods for socp are known to be highly unstable.

## [01199] Recent advances of scientific computing and applications

**Session Time & Room :** 2E (Aug.22, 17:40-19:20) @E508

**Type :** Proposal of Minisymposium

**Abstract :** There has been tremendous growth in various areas of scientific computing in the recent years. This mini-symposium intends to introduce the recent advances of scientific computing and the related interesting applications. The goal is to attract attention to scientific computing and build potential future collaborations.

**Organizer(s) :** Ying Wang

**Classification :** 65M25, 37A50, 92-08

**Minisymposium Program :**

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01199 (1/1) : 2E @E508

## [04888] Plant virus propagation models with delay and stochasticity

**Author(s) :** Benito Chen-Charpentier (University of Texas at Arlington)

**Abstract :** Plant diseases caused by a virus are mostly transmitted by a vector that bites an infected plant and bites a susceptible one. There is a delay between the time a plant gets bitten by an infected vector and the time it is infected. In this paper we consider two simple models of plant virus propagation and study different ways in which delays can be incorporated including the addition of an exposed class for the plants. Simulations are done and comparisons with the results for the models without delays are presented.

## [05157] Numerical studies to the Chaplygin gas equation

**Author(s) :** Ying Wang (University of Oklahoma)

**Abstract :** In this talk, we will discuss the numerical solutions to the Riemann problem for Chaplygin gas equation, which is the Euler equations equipped with the state equation  $p = -1/\rho$ . The spatial discretization is performed using WENO reconstruction and time integration is achieved using TVD RK4. The numerical results confirm high order of accuracy. This is a joint work with Ling Jin.

## [05160] Fully coupled averaging with singularities.

**Author(s) :** Alexander Grigo (University of Oklahoma)

**Abstract :** In this talk I will present an averaging theorem for a fully coupled system with singularities. Specifically, I will discuss a particular fast-slow system that arises in modeling energy transport in an open system of interacting hard-spheres. The technical part of this work addresses how to deal with singularities of the dynamics and the fact that the dynamics is fully coupled.

## [01200] New Trends in Optimal Control and Their Applications

**Session Time & Room :**

01200 (1/2) : 1C (Aug.21, 13:20-15:00) @F312

01200 (2/2) : 1D (Aug.21, 15:30-17:10) @F312

**Type** : Proposal of Minisymposium

**Abstract** : This proposal belongs to the area of optimal control for sweeping processes and their applications to optimization-related and control problems, as well as some practical models. By now, the sweeping process has been recognized as a class of nonsmooth dynamical systems involving normal cones to moving sets. The controlled sweeping processes have been studied with applications relating to the theory of plasticity, ferromagnetism, ferroelectricity, and elastoplasticity. Further developments also apply to various problems of hysteresis, phase transitions, modelling systems with contact, friction, and impacts. These systems frequently arise in applications such as mechanical systems, switched electrical circuits, and biological systems.

**Organizer(s)** : Leonardo Colombo, Dao Nguyen

**Classification** : 47J20, 49J40, 49J53, 65K10, 90C99

**Minisymposium Program** : No registered information

## [01202] Analysis and modelling of human flows

**Session Time & Room** : 4E (Aug.24, 17:40-19:20) @G302

**Type** : Proposal of Minisymposium

**Abstract** : People are moving from one location to another in their daily lives, for commuting, shopping, entertainment, schools, etc. This human flow provides vital information for location decision-making for commercial or public buildings, optimization of transportation systems, urban planning by policymakers, and measures for movement restrictions under a pandemic like COVID-19. This mini-symposium will discuss recent developments in the modeling and analysis of human mobility from an interdisciplinary perspective, including urban studies, spatial economics, network science, and applied mathematics.

**Organizer(s)** : Takaaki Aoki and Naoya Fujiwara

**Classification** : 05C21

**Minisymposium Program** :

01202 (1/1) : 4E @G302 [Chair: Takaaki Aoki]

## [03707] Recent Public Data Related with Urban Vehicle Traffic Simulation

**Format** : Talk at Waseda University

**Author(s)** : Takeshi Uchitane (Aichi Institute of Technology)

**Abstract** : Various kinds of social data are available in Japan in order to realize and evaluate vehicle simulations within an urban-scale digital map. In such the social data, open data is becoming more and more common. In our discussion, two case studies of vehicle simulations and related open data are explained. Because the target locations are different between Kobe city and Aichi prefecture, different kinds of open data are required to make appropriate origin-destination pairs.

## [04718] Urban scale pedestrian simulation and analysis around Kobe City center

**Format** : Talk at Waseda University

**Author(s)** : Daigo Umemoto (RIKEN R-CCS)Maiko Kikuchi (NTT DOCOMO, INC)Ayako Terui (NTT DOCOMO, INC)Koutarou Abe (NTT DOCOMO, INC)Ryuushi Shimizu (NTT DOCOMO, INC)Katsuki Hirashige (NTT DOCOMO, INC)Nobuyasu Ito (RIKEN R-CCS)Itsuki Noda (Hokudai)

**Abstract** : We constructed a pedestrian evacuation simulator for Kobe City center, using population based on cell phone demographics provided by NTT DoCoMo, Inc., pedestrian simulator CrowdWalk, and Open Street Map with manually added signals. The evacuation time was initially simulated as 25,685 seconds. Decentralizing evacuation routes reduced it to 17,780 seconds. The signal removal further reduced it to 9,550 seconds. The signal removal alone gave 12,475 seconds: interestingly, overall reduction was about 50% in both cases.

## [02895] Potential field of human flow extracted by Hodge-Kodaira decomposition

**Format :** Talk at Waseda University

**Author(s) :** Takaaki Aoki (kagawa university, japan)Shota Fujishima (Hitotsubashi University)Naoya Fujiwara (Tohoku University)

**Abstract :** People are moving daily from one location to another for commuting, shopping, entertainment, schools, etc. Human movements provide vital information for unfolding the actual shapes of cities. Here, we show the potential of human flows using the orthogonal decomposition of the combinatorial Hodge theory for the origin-destination matrix. The potential landscape visualizes an intuitive perspective of the urban structure behind the massive movements and helps us examine the complex spatial structures in contemporary metropolitan areas.

## [03549] Towards science of multi-scale human flow

**Format :** Talk at Waseda University

**Author(s) :** Naoya Fujiwara (Tohoku University)

**Abstract :** In this talk, we present our recent findings in data analysis and mathematical models of human mobility, with an emphasis on characteristics of different temporal and spatial scales. The examples include data analysis of evacuation behaviors for severe disasters, change in the mobility patterns after COVID-19 pandemic, and mathematical models for long-term migration patterns. These results would provide hints to obtain a general framework for studying and understanding human mobility.

# [01211] Generalized and non-Gaussian Tensor Decompositions

**Session Time & Room :**

01211 (1/2) : 1C (Aug.21, 13:20-15:00) @G306

01211 (2/2) : 1D (Aug.21, 15:30-17:10) @G306

**Type :** Proposal of Minisymposium

**Abstract :** Tensor decompositions are a foundational unsupervised machine learning method for data science, with applications across all of science and engineering. Traditionally, tensor decompositions seek low-rank tensors that best fit the data with respect to the least squares loss. However, other choices of loss function can be more appropriate for non-Gaussian data such as count data, binary data, and data with outliers. This minisymposium presents state-of-the-art advances in developing efficient algorithms and rigorous theory for tensor decompositions with respect to general losses.

**Organizer(s) :** David Hong

**Classification :** 15A69

**Minisymposium Program :**

01211 (1/2) : 1C @G306 [Chair: David Hong]

## [05616] Generalized Canonical Polyadic Tensor Decomposition: Algorithms and Applications

**Format :** Talk at Waseda University

**Author(s) :** David Hong (University of Delaware)

**Abstract :** Canonical polyadic (CP) tensor decomposition is a fundamental method for finding underlying patterns in data tensors by fitting a low-rank tensor to the data with respect to the least-squares loss. This talk gives an introduction to the generalized CP (GCP) tensor decomposition, which allows general user-selected losses (i.e., non-Gaussian/non-Euclidean/non-least-squares losses). We will describe first-order algorithms for computing GCP and show various demonstrations of GCP on data from science and engineering.

## [05224] Recent Improvements in CP Poisson Tensor Algorithms

**Format :** Online Talk on Zoom

**Author(s) :** Jeremy Myers (Sandia National Laboratories) Daniel Dunlavy (Sandia National Laboratories)

**Abstract :** The challenge of fitting a low-rank, non-negative canonical polyadic tensor model to Poisson-distributed multi-way data is often formulated as a nonconvex optimization problem. A common approach is to use local methods initialized from many random starting points to improve the probability of convergence to the global minimum, which is costly. Our mitigation is a heuristic that identifies and teleports away from suboptimal solutions to improve the probability of convergence and reduce computational cost.

## [04808] Second-order algorithms for canonical polyadic decomposition with non-least-squares cost functions

**Format :** Talk at Waseda University

**Author(s) :** Michiel Vandecappelle (Televis Rail NV) Nico Vervliet (KU Leuven) Lieven De Lathauwer (KU Leuven)

**Abstract :** Signal processing and data analysis applications often rely on rank-1 terms to extract meaningful information from tensor data. By using the least-squares loss when computing this canonical polyadic decomposition, one implicitly assumes normally distributed errors, which might not be suitable for, e.g., count data. Therefore, we derive a generalized Gauss-Newton-type algorithm for non-least-squares loss functions and discuss how exploiting tensor structure and randomization lead to an efficient algorithm.

## [05553] Efficient Algorithms and Software for Generalized Tensor Completion

**Format :** Online Talk on Zoom

**Author(s) :** Navjot Singh (University of Illinois Urbana-Champaign) Edgar Solomonik (University of Illinois at Urbana-Champaign)

**Abstract :** We present novel algorithms and systems infrastructure which enable efficient parallel implementation of algorithms for CP tensor completion with generalized loss functions.

Specifically, we consider alternating minimization, coordinate minimization, and a quasi-Newton (generalized Gauss-Newton) method.

By extending the Cyclops library, we implement all these methods in high-level Python syntax using new sparse tensor kernels. We demonstrate the generalizability of our framework with the first large-scale implementation for Poisson loss completion.

01211 (2/2) : 1D @G306 [Chair: David Hong]

## [03326] Stochastic Mirror Descent for Low-Rank Tensor Decomposition Under Non-Euclidean Losses

**Format :** Talk at Waseda University

**Author(s) :** Wenqiang PU (Shenzhen Research Institute of Big Data) Xiao FU (Oregon State University)

**Abstract :** This talk considers low-rank canonical polyadic decomposition (CPD) under a class of non-Euclidean loss functions that frequently arise in statistical machine learning and signal processing. These loss functions are often used for certain types of tensor data, e.g., count and binary tensors, where the least squares loss is considered unnatural. Compared to the least squares loss, the non-Euclidean losses are generally more challenging to handle. Non-Euclidean CPD has attracted considerable interests and a number of prior works exist. However, pressing computational and theoretical challenges, such as scalability and convergence issues, still remain. This talk offers a unified stochastic algorithmic framework for large-scale CPD decomposition under a variety of non-Euclidean loss functions. Our key contribution lies in a tensor fiber sampling strategy-based flexible stochastic mirror descent framework. Leveraging the sampling scheme and the multilinear algebraic structure of low-rank tensors, the proposed lightweight algorithm ensures global convergence to a stationary point under reasonable conditions. Numerical results show that our framework attains promising non-Euclidean CPD performance. The proposed framework also exhibits substantial computational savings compared to state-of-the-art methods.

## [03666] Generalized Tucker tensor estimation: An optimal statistical and computational framework

**Format :** Online Talk on Zoom

**Author(s) :** Anru Zhang (Duke University) Rungang Han (Duke University) Rebecca Willett (University of Chicago)

**Abstract :** We describe a flexible framework for generalized low-rank tensor estimation problems. The proposed estimator consists of finding a low Tucker rank tensor fit to the data under generalized parametric models. To overcome the difficulty of nonconvexity, we introduce a unified approach of projected gradient descent. We establish both an upper bound on the statistical error and the linear rate of computational convergence. We demonstrate the superiority of the proposed framework on real data.

## [01218] Challenges in single-cell data science: theory and application

**Session Time & Room :**

01218 (1/3) : 4E (Aug.24, 17:40-19:20) @E804

01218 (2/3) : 5B (Aug.25, 10:40-12:20) @E804

01218 (3/3) : 5C (Aug.25, 13:20-15:00) @E804

**Type :** Proposal of Minisymposium

**Abstract :** Single-cell data science aims to understand cells and their functions at individual cells and accelerate progress in the biomedical sciences via the analysis of single-cell omics data. The largest hurdle to this is the difficulty of extracting complex biological structures from millions of pieces of information across varied cell data. This mini-symposium focuses on theoretical studies of single-cell data analysis and its applications, in which biologists, applied mathematicians, and bioinformaticians working in single-cell data science worldwide will come together to discuss their research and the future development.

**Organizer(s) :** Yusuke Imoto, Keita Iida, Kazumitsu Maehara

**Classification :** 68T09, 68-11, 92B20, Single-cell data science

**Minisymposium Program :**

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01218 (1/3) : 4E @E804 [Chair: Yusuke Imoto]

## [03514] Resolution of the curse of dimensionality in single-cell RNA sequencing data analysis

**Format :** Talk at Waseda University

**Author(s) :** Yusuke Imoto (Kyoto University)

**Abstract :** We have developed a novel noise reduction method for single-cell RNA sequencing (scRNA-seq) data, RECODE, to resolve the curse of dimensionality (COD) in high-dimensional data analysis. RECODE can reduce technical noises in scRNA-seq data based on high-dimensional statistics theory. In this talk, we will explain biological verification, applicability, and recent progress of RECODE. Moreover, we will overview mathematical/informatical grand challenges in single-cell data science, which is the theme of this minisymposium, at the beginning.

## [05223] Trajectory inference framework by entropic Gaussian mixture optimal transport

**Format :** Talk at Waseda University

**Author(s) :** Toshiaki Yachimura (Tohoku University)

**Abstract :** In 1957, C.H. Waddington introduced the epigenetic landscape for cell differentiation. Recently, many attempts have been made to reconstruct this conceptual model from gene expression data. In this talk, I will introduce scEGOT, a novel trajectory inference framework of cell differentiation for time series scRNA-seq data based on Entropic Gaussian mixture optimal transport. scEGOT allows us to infer the dynamics of gene expression associated with cell differentiation. This talk is based on the WPI-ASHBi project.

## [03619] Dissecting cell identity via network inference and in-silico gene perturbation

**Author(s)** : Kenji Kamimoto (Washington University in St.Louis)

**Abstract** : Single-cell omics technology enables the acquisition of multi-dimensional data in a high-throughput manner, revealing diverse and heterogeneous cellular identities. However, understanding biological events from a gene regulatory networks (GRNs) perspective remains difficult. Here, we have developed a new method, CellOracle, for the inference and analysis of GRNs. The method can perform in silico transcription factor perturbations, simulating the consequent changes in cell identity and promoting new mechanistic insights into the regulation of cell identity.

## [03878] Experimental guidance for discovering genetic networks from time series

**Format** : Talk at Waseda University

**Author(s)** : Tomas Gedeon (Montana State University)Breschne Cummins (Montana State University)Steve Haase (Duke University)Konstantin Mischaikow (Rutgers University)

**Abstract** : We describe an iterative network hypothesis reduction from time-series data in which dynamic expression of individual, pairs, and entire collections of genes are used to infer core network models. The result of our work is a computational pipeline that prioritizes targets for genetic perturbation to experimentally infer network structure. We apply this computational pipeline to synthetic and yeast cell-cycle data.

01218 (2/3) : 5B @E804 [Chair: Kazumitsu Maehara]

## [03512] Geometry-aware high-dimensional vector field reconstruction using Hodge decomposition

**Format** : Talk at Waseda University

**Author(s)** : Kazumitsu Maehara (Kyushu University)

**Abstract** : We propose a method based on Hodge decomposition for analyzing high-dimensional and complex molecular dynamics using single-cell omics data. Drawing inspiration from topology and differential geometry, we developed a data-driven vector field reconstruction method that smoothly captures key features of dynamics (e.g., potential, divergence, curl, and Jacobian) with reduced computational costs through appropriate connections and regularization. Our approach has the potential to contribute to biological discoveries and understanding.

## [03922] Reconstructing single cell dynamics on graphs

**Format** : Talk at Waseda University

**Author(s)** : Jianhua Xing (University of Pittsburgh)

**Abstract** : Single-cell (sc)RNA-seq, together with RNA velocity and metabolic labeling, reveals cellular states and transitions at unprecedented resolution. A frontier of research is how to extract dynamical information from the snapshot data. I will first discuss our recently developed dynamo framework (Qiu et al. Cell, 2022), focusing on the underlying mathematical framework. Then I will discuss our recent efforts of reconstructing full dynamical equations using discrete calculus on graphs (Zhang et al. to be submitted).

## [04897] Deep generative models to reveal cellular level dynamics and communication

**Format** : Talk at Waseda University

**Author(s)** : Teppei Shimamura (Tokyo Medical and Dental University)

**Abstract** : In this talk, we present a deep generative model for investigating the dynamic changes and interactions between cells that alter various states during the onset and progression of diseases from single-cell and spatial omics data.

01218 (3/3) : 5C @E804 [Chair: Keita Iida]

## [03515] Functional annotation-driven unsupervised clustering for single-cell data

**Format :** Talk at Waseda University

**Author(s) :** Keita Iida (Osaka University)

**Abstract :** Single-cell and spatial transcriptomics have enhanced our knowledge of molecular complexity in terms of gene expression heterogeneity in cell populations. However, conventional gene-based approaches may be insufficient in capturing such complexity as genes can interact with each other to regulate a number of biological functions. Here, we introduce ASURAT, a computational tool for simultaneous clustering and functional annotation of single-cell and spatial transcriptomes in terms of cell type, disease, biological process, and signaling pathway activity.

## [03908] Modelling cell differentiation: from psuedo-time to energy landscape

**Format :** Online Talk on Zoom

**Author(s) :** Jifan Shi (Fudan University)

**Abstract :** Interactions between genes determine cell development and differentiation. We first introduce pseudo-time of cells, which is also known as pluripotency. Next, we will focus on models from the perspective of energy landscape. We propose an energy landscape decomposition theory for cell differentiation with proliferation effect. Two energy landscapes collectively contribute to the establishment of non-equilibrium steady differentiation. We will also demonstrate feasible numerical methods and several interesting applications.

## [03682] Integrating data and dynamics in scRNA-seq data analysis

**Format :** Talk at Waseda University

**Author(s) :** Tiejun Li (Peking University)

**Abstract :** In this talk, I will review some research progress of my group on the scRNA-seq data analysis in recent years. I will mainly focus on the integration of data and dynamics approach in this area, which includes the theory and algorithms for the RNA velocity, dynamical approach for the scRNA-seq data with temporal information, and deep learning type methods. This is a series of joint works with Prof. Luonan Chen, Qing Nie, and Dr. Peijie Zhou, Jifan Shi, Yichong Wu, Qiangwei Peng, et al.

## [01221] FreeFEM software package for finite element modeling of PDEs

**Session Time & Room :** 2E (Aug.22, 17:40-19:20) @E504

**Type :** Proposal of Minisymposium

**Abstract :** FreeFEM is a software package for finite element computation and has been developing at the Laboratory of Jacques-Louis Lions, Sorbonne University for 25 years. The main feature of FreeFEM is having a domain specific language based on C++ grammar, which is designed to describe variational formulation of the partial differential equations and discretized matrices by using numerical quadrature on triangle and tetrahedral elements. Now it is drastically enhanced to perform large scale three dimensional computation using domain decomposition methods by linking with tetrahedral mesh generators and parallel linear solvers. FreeFEM allows us to tackle a new mathematical modeling and solution by expressing nonlinear weak formulation with surface and domain integration and by direct manipulation of finite element matrices. This mini-symposium focuses on recent advancement of FreeFEM and application in mathematical modeling.

**Organizer(s) :** Atsushi Suzuki, Takeshi Takaishi

**Classification :** 65-04, 65Fxx, 65Kxx, 65N30

**Minisymposium Program :**

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01221 (1/1) : 2E @E504 [Chair: Atsushi Suzuki]

## [02183] Phase field crack growth simulation using IPOPT package

**Format :** Talk at Waseda University

**Author(s) :** Takeshi Takaishi (Musashino University)

**Abstract :** As the energy gradient flow equation of the Bourdin model, we introduced the time evolution model of irreversible crack growth by the phase field method. Its weak solution can be written in terms of variational inequalities, since it includes the irreversible crack state. Simulation results for this model with the IPOPT package in FreeFEM shows the energy dissipation process of crack growth precisely.

## [02252] Direct factorization of indefinite matrix for constrained problem in finite element modeling

**Format :** Talk at Waseda University

**Author(s) :** Atsushi Suzuki (RIKEN Center for Computational Science)

**Abstract :** Finite element computation of some physical problem with constraint uses a variational problem with Lagrange multipliers as dual variables. Physical constraints are supposed as incompressibility of the fluid, boundary conditions on internal interfaces, and so on. A linear system obtained by a discretization becomes indefinite and then the multifrontal method for parallelization of direct methods may suffer pseudo singularity of subproblems. Careful pivoting with keeping pair of primal and dual unknowns makes the factorization stable.

## [02281] An easy-to-use framework for the density-based topology optimization of multiphysics systems written in FreeFEM-PETSc-ParMmg

**Format :** Talk at Waseda University

**Author(s) :** Hao Li (Kyoto University)Minghao Yu (China Academy of Engineering Physics)Pierre Jolivet (LIP6, Sorbonne Universite)Joe Alexandersen (University of Southern Denmark)Atsushi Suzuki (Osaka University)Shinji Nishiwaki (Kyoto University)

**Abstract :** Large-scale 3D topology optimization has been a big trend in the previous decade. However, it features a high computational cost, which may not always be available to general users. We constructed an easy-to-use and fully distributed framework written in FreeFEM-PETSc-ParMmg. We present various 2D and 3D benchmarks including a structural problem, a transient thermal cloaking design, and a thermal-fluidic problem.

## [02204] Recent advances with FreeFEM in parallel and its interface to PETSc

**Format :** Talk at Waseda University

**Author(s) :** Pierre Jolivet (CNRS)

**Abstract :** In this talk, I will present some new features of FreeFEM and its interface to PETSc and SLEPc. Coupled together, these libraries offer a flexible infrastructure to deal with coupled and/or high-dimensional systems, using MPI for distributed-memory parallelism. I will showcase some examples from fluid dynamics, radiative transfer, and boundary integral equations.

## [01229] Cauchy problem for Deterministic and Stochastic nonlinear dispersive equations

**Session Time & Room :** 5C (Aug.25, 13:20-15:00) @G709

**Type :** Proposal of Minisymposium

**Abstract :** We consider Cauchy problem for Deterministic and Stochastic nonlinear dispersive equations. For the Deterministic nonlinear Schrödinger equation (NLS), some global dynamics will be discussed, that is scattering, blowing up, growing up, or uniform bound for the solutions of NLS. For the Stochastic NLS, we will deal with nonlinear equation with a multiplicable noise. We also introduce and discuss paracontrolled calculus to prove local well-posedness of a renormalized version of the stochastic nonlinear wave equation.

**Organizer(s) :** Shuji Machihara

**Classification :** 35Q55, 60H15, 60H40**Minisymposium Program :**

01229 (1/1) : 5C @G709 [Chair: Shuji Machihara]

## [03890] The well-posedness of the stochastic nonlinear Schrödinger equations in $H^2$

**Format :** Talk at Waseda University**Author(s) :** Shunya Hashimoto (Saitama university)

**Abstract :** We consider the well-posedness of  $H^2$ -solutions in initial value problems for the stochastic nonlinear Schrödinger equations with power-type nonlinear terms with multiplicative noise. For the proof, we use the rescaling approach, which transforms the stochastic equation into a random equation in which no white noise appears. Unlike  $L^2$ - and  $H^1$ -solution, there are two difficulties in the  $H^2$ -solution: first, the lack of the smoothness of nonlinear functions, and second, the treatment of white noise that reappears.

## [04966] Time behavior of solutions to nonlinear Schrödinger equation with a potential

**Format :** Talk at Waseda University**Author(s) :** Masaru Hamano (Waseda University)

**Abstract :** In this talk, we deal with the Cauchy problem of a nonlinear Schrödinger equation with a potential. In particular, we consider time behavior of solutions to the equation with initial data, whose energy is equal to that of the Talenti function.

## [03584] Well-posedness for the fourth-order Schrödinger equation with third order derivative nonlinearities

**Format :** Talk at Waseda University**Author(s) :** Noriyoshi Fukaya (Tokyo University of Science)

**Abstract :** We study the Cauchy problem to the semilinear fourth-order Schrödinger equations with third order derivative nonlinearities.

The purpose of this presentation is to prove well-posedness of the problem in the lower order Sobolev space  $H^s(\mathbb{R})$  or with more general nonlinearities than previous results. Our proof of the main results is based on the contraction mapping principle on a suitable function space employed by D. Pornnoppaphat (2018). To obtain the key linear and bilinear estimates,

we construct a suitable decomposition of the Duhamel term introduced by I. Bejenaru, A. D. Ionescu, C. E. Kenig, and D. Tataru (2011). Moreover we discuss scattering of global solutions and the optimality for the regularity of our well-posedness results, namely we prove that the flow map is not smooth in several cases.

## [05020] Convergence of the intermediate long wave equation from a statistical perspective

**Format :** Talk at Waseda University**Author(s) :** Guopeng Li (The Maxwell Institute for Mathematical Sciences)

**Abstract :** The intermediate long wave equation (ILW) models water waves of finite depth, connecting the Benjamin-Ono equation (deep-water limit) and the KdV equation (shallow-water limit). Convergence problems of ILW (in both the deep-water and shallow-water limits) have attracted attention from both the applied and theoretical points of view. In this talk, I will discuss convergence problems from a statistical viewpoint. I first consider the convergence problem of the Gibbsian ensembles. In this case, I establish convergence of the Gibbs measures and then also show convergence of invariant Gibbs dynamics to that of the Benjamin-Ono and KdV equations (without uniqueness).

ILW is known to be completely integrable and thus possesses infinitely many conservation laws. In the second part of the talk, I consider invariant dynamics for ILW associated with higher order conservation laws. Due to a complicated nature of the dispersion, even the construction of measures associated with higher order conservation laws turns out to be highly non-trivial. By considering a suitable combination of higher order conservation laws, I overcome this issue and construct invariant dynamics for ILW with a fixed depth parameter. In the final part, I will discuss convergence of the invariant dynamics associated with higher order conservation laws.

This talk is based on a joint work with Tadahiro Oh (Edinburgh), Guangqu Zheng (Liverpool), and Andreia Chapouto (UCLA).

## [01272] Interface motion and related topics

### **Session Time & Room :**

01272 (1/2) : 4D (Aug.24, 15:30-17:10) @G710

01272 (2/2) : 4E (Aug.24, 17:40-19:20) @G710

**Type :** Proposal of Minisymposium

**Abstract :** Understanding the interface dynamics, such as in crystal growth and moving boundaries between two phases, is a topic of great mathematical interest and is also important from engineering, materials science, and other perspectives.

This mini-symposium aims to bring together researchers working on interfacial motion and related topics to share recent advances and discuss this domain of interest.

Topics to be presented include mathematical analysis of interface behavior, numerical methods specific to interface motion, and applied research such as the shape optimization.

**Organizer(s) :** Michal Beneš, Tetsuya Ishiwata

**Classification :** 35R35, 65N99, 76D27

### **Minisymposium Program :**

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01272 (1/2) : 4D @G710 [Chair: Michal Beneš]

## [02736] Numerical computation of the Plateau problem by the method of fundamental solutions

**Format :** Talk at Waseda University

**Author(s) :** Koya Sakakibara (Okayama University of Science / RIKEN)Yuuki Shimizu (The University of Tokyo)

**Abstract :** We propose a numerical scheme for the Plateau problem based on the method of fundamental solutions. After giving the existence of approximate surfaces and convergence analysis, some numerical experiments show the usefulness of the proposed scheme.

## [04050] Novel numerical methods for solving nonlinear evolutionary equations with application in mathematical finance optimization problems

**Format :** Talk at Waseda University

**Author(s) :** Cyril Izuchukwu Udeani (Comenius University in Bratislava)Daniel Sevcovic (Comenius University)

**Abstract :** This study employs physics-informed DeepONet (PI-DeepONet), which incorporates known physics into the neural network via two networks, to approximate the solution operator of a nonlinear Hamilton-Jacobi-Bellman (HJB) equation arising from the stochastic optimization problem, where an investor's goal is to maximize the conditional expected value of the terminal utility. We first transform the nonlinear HJB equation into a quasilinear parabolic equation using the Riccati transform and then approximate the solution of the transformed equation using PI-DeepONet.

## [02939] Mathematical modeling of flame/smoldering front-evolution and its application

**Format :** Talk at Waseda University

**Author(s) :** Shunsuke Kobayashi (University of Miyazaki)Shigetoshi Yazaki (Meiji University)Kazunori Kuwana (Tokyo University of Science)

**Abstract :** The Kuramoto-Sivashinsky equation is well-known as a mathematical model describing the interfacial dynamics of combustion phenomena. In this talk, we focus on flame spreading over thin solid fuels and report the results of applying the Kuramoto-Sivashinsky equation to the following two topics:

1. the behavior of flame/smoldering fronts expanding circle with time.
2. the spreading speed of flame front in a spatially non-uniform region with a bellows shape.

## [04059] Multidimensional partial integro-differential equation in Bessel potential spaces with applications

**Format :** Talk at Waseda University

**Author(s) :** Daniel Sevcovic (Comenius University)Cyril Izuchukwu Udeani (Comenies University)

**Abstract :** In the talk we analyze solutions of a non-local nonlinear partial integro-differential equation (PIDE) in multidimensional spaces. We employ the theory of abstract semilinear parabolic equations in order to prove existence and uniqueness of solutions in the scale of Bessel potential spaces. We prove existence and uniqueness of a solution to the PIDE. As an application to option pricing in the one-dimensional space, we consider a general shift function arising from nonlinear option pricing models.

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01272 (2/2) : 4E @G710 [Chair: Tetsuya Ishiwata]

## [04426] Qualitative and numerical aspects of dynamics of diffusion and transport mechanisms on evolving curves

**Format :** Talk at Waseda University

**Author(s) :** Miroslav Kolar (Czech Technical University in Prague)

**Abstract :** In this talk we discuss the model of diffusion and transport acting on evolving curves. The model is coupled with the geometrical evolution equation for moving interfaces in form normal velocity = curvature + force. This model is being developed within the context of study of the vortex dynamics. The technique of incorporation an artificial tangential velocity for the stabilisation of numerical calculations is discussed and qualitative and quantitative computational results in 2D and 3D are shown.

## [02845] Numerical solution to a free boundary problem for the Stokes equation using the coupled complex boundary method in shape optimization settings

**Format :** Talk at Waseda University

**Author(s) :** Julius Fergy Tiongan Rabago (Kanazawa University)Hirofumi Notsu (Kanazawa University)

**Abstract :** A new reformulation of a free boundary problem for the Stokes equations governing a viscous flow is proposed. Using the shape derivative of the cost associated with the new cost functional, a Sobolev-gradient based descent method is employed to solve the shape optimization problem. For validation and evaluation of the method, numerical experiments are carried out both in two and three dimensions which are compared with the ones obtained via the classical Dirichlet-data tracking approach.

## [03222] Structure-preserving numerical methods for gradient flows of planar closed curves

**Format :** Talk at Waseda University

**Author(s) :** Tomoya Kemmochi (Nagoya University)Yuto Miyatake (Osaka University)Koya Sakakibara (Okayama University of Science)

**Abstract :** In this talk, we consider numerical approximation of constrained gradient flows of planar closed curves. We will develop structure-preserving methods for these equations that preserve both the dissipation and the constraints. To preserve the energy structures, we introduce the discrete version of gradients according to the discrete gradient method and determine the Lagrange multipliers appropriately. Some numerical examples are presented to verify the efficiency of the proposed schemes.

## [02751] Motion of Space Curves by Binormal and Normal Curvature

**Format :** Talk at Waseda University

**Author(s) :** Michal BENES (Faculty of Nuclear Sciences and Physical Engineering, Czech Technical University in Prague)Miroslav KOLÁŘ (Faculty of Nuclear Sciences and Physical Engineering, Czech Technical University in Prague)Daniel ŠEVČOVIČ (Faculty of Mathematics, Physics and Computer Science, Comenius University in Bratislava)

**Abstract :** We discuss the motion of closed non-intersecting space curves by curvature in binormal and normal directions with application in vortex dynamics. We formulate the general motion law in space by binormal and normal curvature and mention its analytical properties. The finite-volume scheme allows to solve the motion part\_2

numerically with stabilization by the tangential velocity redistributing discretization nodes. We demonstrate behavior of the solution on several computational studies combining normal and binormal velocity and mutual interactions.

## [01383] Sustainable Logistics and Transportation under Uncertain Environments

**Session Time & Room :** 3D (Aug.23, 15:30-17:10) @D505

**Type :** Proposal of Industrial Minisymposium

**Abstract :** Sustainable logistics mention the processes and practices aimed at enriching sustainability of supply chain operations, starting from supply of raw materials to transferring process, storage, packaging, distributions, and customers at the end of life cycle of items. Logistics and transportation problems are examined within a sustainability perspective to offer a comprehensive assessment of economical, environmental, and social performance measures. Sustainable logistics and transportation under uncertain environments provide an appropriate idea for many authorities and decision-makers.

**Organizer(s) :** Sankar Kumar Roy

**Classification :** 90B06, 90C70

**Minisymposium Program :** No registered information

## [01445] Deep Learning, Preconditioning, and Linear Solvers

**Session Time & Room :**

01445 (1/2) : 5C (Aug.25, 13:20-15:00) @E507

01445 (2/2) : 5D (Aug.25, 15:30-17:10) @E507

**Type :** Proposal of Minisymposium

**Abstract :** The numerical solution of linear systems of equations is the computational bottleneck in a whole spectrum of applied mathematics and computational science problems. Recently, a number of works have investigated how deep learning can accelerate this critical solution process. This minisymposium will showcase cutting-edge innovations in using deep learning techniques to design and accelerate preconditioners and solvers for linear systems. Researchers will share recent work on topics like combining neural networks with multigrid solvers or conjugate direction methods. An emphasized application will be large, sparse linear systems that arise from discretized partial differential equations in computational physics and simulation problems.

**Organizer(s) :** David Hyde

**Classification :** 65F08, 65F10, 65T07, 65N22

**Minisymposium Program :**

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01445 (1/2) : 5C @E507 [Chair: David Hyde]

## [03314] Deep Learning, Preconditioning, and Linear Solvers

**Format :** Talk at Waseda University

**Author(s) :** David Hyde (Vanderbilt University)

**Abstract :** We will survey techniques for using learning to accelerate linear solvers and preconditioners. Some methods use learning to determine high-quality initial guesses for iterative systems; other approaches learn parameters for classical preconditioners like algebraic multigrid; further techniques replace the entire role of a preconditioner with learning; and still other works replace entire linear solvers with neural network evaluations. After surveying these approaches, we will suggest some avenues of research, open questions, and opportunities for collaboration.

## [04332] Fourier Neural Solver for Large Sparse Linear Algebraic Systems

**Format :** Talk at Waseda University

**Author(s) :** Kai Jiang (Xiangtan University)

**Abstract :** In this talk, we propose an interpretable neural solver, the Fourier neural solver (FNS), to solve sparse linear algebraic systems. Based on deep learning and fast Fourier transformation, FNS combines a stationary iterative method and frequency space correction approach to efficiently eliminate different frequency components of the error. The local Fourier analysis indicates that FNS can detect error components within the frequency domain that cannot be eliminated effectively using stationary methods, even though the error removed by the latter is problem-dependent. Numerical experiments on several classical equations show that the FNS is more efficient and more robust than the existing neural solvers. If time permits, we will update our latest progress in this area.

## [03199] Accelerating multigrid solvers for the acoustic and elastic Helmholtz equation.

**Format :** Talk at Waseda University

**Author(s) :** Rachel Yovel (Ben-Gurion University of the Negev)Eran Treister (Ben-Gurion University of the Negev)Bar Lerer (Ben-Gurion University of the Negev)

**Abstract :** We develop multigrid solvers for the acoustic and elastic Helmholtz equations and accelerate them using deep learning methods. Based on the shifted Laplacian approach, which is typically used for the acoustic version, we build a GPU-friendly geometric multigrid preconditioner for the elastic Helmholtz equation. Moreover, we present a block-acoustic preconditioner for the elastic version and utilize a trained CNN acoustic solver to solve the elastic Helmholtz equation through this reduction.

## [03141] On learning neural operators of PDEs with interfacial jump conditions for accelerating simulations of physical systems

**Format :** Talk at Waseda University

**Author(s) :** Pouria Akbari Mistani (NVIDIA Corp)Samira Pakravan (University of California Santa Barbara)Frederic Gibou (University of California Santa Barbara)

**Abstract :** Elliptic (free boundary) problems with jump conditions are commonly used to model multiscale physical systems. Despite the availability of optimal numerical solvers, obtaining solutions over large spatiotemporal scales remains challenging. Pre-trained compact neural operators offer fast inference oracles to accelerate simulations on modern hardware. In this talk we present our work on training accurate neural operators for this class of problems. We also introduce JAX-DIPS, a publicly available library, to promote research in this area.

01445 (2/2) : 5D @E507 [Chair: David Hyde]

## [03614] A Deep Conjugate Direction Method for Iteratively Solving Linear Systems

**Format :** Talk at Waseda University

**Author(s) :** ayano kaneda (waseda university)David Hyde (Vanderbilt University)Osman Aker (University of California)Joseph Teran Michael ( University of California, Davis)

**Abstract :** We present a novel deep learning approach to approximate the solution of large, sparse, symmetric, positive-definite linear systems of equations. Motivated by the conjugate gradients algorithm that iteratively selects search directions for minimizing the matrix norm of the approximation error, we design an approach that utilizes a deep neural network to accelerate convergence via data-driven improvement of the search direction at each iteration. Our method leverages a carefully chosen convolutional network to approximate the action of the inverse of the linear operator up to an arbitrary constant. We demonstrate the efficacy of our approach on spatially discretized Poisson equations, which arise in computational fluid dynamics applications, with millions of degrees of freedom. Unlike state-of-the-art learning approaches, our algorithm is capable of reducing the linear system residual to a given tolerance in a small number of iterations, independent of the problem size. Moreover, our method generalizes effectively to various systems beyond those encountered during training.

## [03251] Wasserstein GAN and Transfer Learning in physics-informed neural networks

**Format :** Talk at Waseda University

**Author(s) :** Yihang Gao (The University of Hong Kong) Michael Kwok-Po Ng (The University of Hong Kong)

**Abstract :** We study a physics-informed algorithm for Wasserstein Generative Adversarial Networks (WGANs) for uncertainty quantification in solutions of PDEs. By using groupsort activation functions in adversarial network discriminators, network generators are utilized to learn the uncertainty in solutions of PDEs observed from initial/boundary data. Under mild assumptions, we show the convergence of the obtained model. Moreover, we also study a SVD-based transfer learning method which stabilize the training and reduce the storage for PINNs.

## [01494] Queues and Related Stochastic Models

**Session Time & Room :**

01494 (1/2) : 2D (Aug.22, 15:30-17:10) @E501

01494 (2/2) : 2E (Aug.22, 17:40-19:20) @E501

**Type :** Proposal of Minisymposium

**Abstract :** In this mini-symposium, we invite high-quality contributions in queues and related stochastic models arising from operations research. Queues and related stochastic models have various applications in service systems, such as call centers, computer and communication networks, and transportation systems. This mini-symposium discusses recent advances in queues and stochastic models and their applications.

**Keywords**

- stochastic models
- matrix analytic methods
- asymptotic analysis of queueing models
- game theoretic analysis of queues
- fluid and diffusion limits, large deviation analysis of queues
- stochastic analysis of risk models
- matching queues
- multidimensional Markov chains
- novel queueing models in applications

**Organizer(s) :** Tuan Phung-Duc

**Classification :** 60K25, Queueing Theory, Stochastic Systems, Stochastic Networks

**Minisymposium Program :**

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01494 (1/2) : 2D @E501 [Chair: Tuan Phung-Duc]

## [02929] Strategic revenue management for discriminatory processor sharing queues

**Format :** Talk at Waseda University

**Author(s) :** Dieter Fiems (Ghent University)

**Abstract :** We consider revenue management for discriminatory processor sharing (dps) queues. The server receives revenue per customer, as well as a fee if customers opt for premium service. We study the optimal parameter allocation of the dps discipline, assuming that customers rationally select between premium and non-premium service. It is shown that the optimal dps discipline is a strict priority discipline when customers cannot balk, while a non-degenerate dps discipline is optimal with balking.

## [03027] Bounding performance of stochastic models for server virtualization in cloud computing

**Format :** Talk at Waseda University

**Author(s) :** Ken'ichi Kawanishi (Gunma University)

**Abstract :** In recent years, ICT systems are constructed with virtual servers on the cloud computing by virtualization technology. The cloud computing is based on a huge number of physical servers in data centers. One of the important issues is to reduce server power consumption while ensuring performance. In this talk, we consider stochastic models for server virtualization in cloud computing and propose a method to evaluate performance bounds while suppressing computational costs even in large-scale systems.

## [03114] Strategic behaviour of reserved customers in a queueing model with multiple reservation zones

**Format :** Talk at Waseda University

**Author(s) :** Yutaka Sakuma (Department of Computer Science, National Defense Academy of Japan)Emiko Fukuda (Department of Industrial Engineering and Economics, Tokyo Institute of Technology)Hiroyuki Ichihara (Deptartment of Management Synthesis, Chubu University)Hiroyuki Masuyama (Graduate School of Management, Tokyo Metropolitan University)

**Abstract :** We consider the strategic behavior of customers in a queueing system with multiple reservation zones. In this system, customers are assigned to the reservation zones, and they face the problem of when to arrive within their reservation zone, where early arrival is allowed. The customers are assumed to be homogeneous and non-cooperative, and they try to find a mixed strategy that minimizes their expected waiting time. We propose a numerical algorithm to obtain the customers' mixed strategy in equilibrium for each reservation zone.

## [02958] Analysis of time-dependent queues with generally distributed retrials

**Format :** Talk at Waseda University

**Author(s) :** Raik Stolletz (University of Mannheim)Ömer Özümerzifon (University of Mannheim)Benjamin Legros (EM Normandie)

**Abstract :** Time-dependent queueing systems are present in various service systems. Often customers leave the queue before being served due to a lack of patience. However, impatient users may join the system after the so-called retrial time. We analyze the time-dependent performance of multi-server queues with generally distributed retrial times and develop a stationary backlog-carryover (SBC) approach. The numerical study analyzes the reliability of the approach and demonstrates the impact of retrial time distributions on performance measures.

01494 (2/2) : 2E @E501 [Chair: Tuan Phung-Duc]

## [03351] The rational outcome of queueing games: A fixed-point iteration based approach

**Format :** Talk at Waseda University

**Author(s) :** Hung Q Nguyen (Advanced Artificial Intelligence Innovation Center, Hitachi, Ltd. Research & Development Group)Tuan Phung-Duc (University of Tsukuba)

**Abstract :** In this study, we consider a class of queueing games characterized by the following feature: expected waiting times of enqueued agents are affected by joining strategies of later comers. We survey several queueing models and generalize an iterative algorithm that may universally apply in a class of queueing game problems to computationally solve for the rational outcome of the game.

## [03189] Workload analysis of fluid polling models

**Format :** Online Talk on Zoom

**Author(s) :** Stella Kapodistria (Eindhoven University of Technology)

**Abstract :** In this presentation, we analyze a two-queue random time-limited Markov-modulated polling model. In the first part of the talk, we investigate the fluid version: fluid arrives at the two queues as two independent flows with deterministic rate. There is a single server that serves both queues at constant speeds. The server spends an exponentially distributed amount of time in each queue. After the completion of such a visit time to one queue, the server instantly switches to the other queue, i.e., there is no switch-over time.

For this model, we derive a functional equation for the LST of the two-dimensional workload distribution that leads to a Riemann–Hilbert boundary value problem (BVP). After taking a heavy-traffic limit, and restricting ourselves to the symmetric case, the BVP simplifies and can be solved explicitly.

In the second part of the talk, allowing for more general (Lévy) input processes and server switching policies, we investigate the transient process limit of the joint workload in heavy traffic. Again solving a BVP, we determine the stationary distribution of the limiting process. We show that, in the symmetric case, this distribution coincides with our earlier solution of the BVP, implying that in this case the two limits (stationarity and heavy traffic) commute.

This is joint work with M. Saxena, O.J. Boxma and O. Kella.

## [01532] Recent Trends in Fluid Mechanics and its Applications

### **Session Time & Room :**

01532 (1/2) : 1C (Aug.21, 13:20-15:00) @G704

01532 (2/2) : 1D (Aug.21, 15:30-17:10) @G704

**Type :** Proposal of Minisymposium

**Abstract :** The aim of this minisymposium is to bring together mathematicians to share their recent progress and to inspire new ideas in applied mathematics.

This minisymposium may address modeling various phenomenon arising from gas dynamics, astrophysics, engineering, and material science, as well as theoretic analysis in problems of kinetic theory, planetary atmospheric science, traffic flow, and semiconductor etc.

**Organizer(s) :** Shih-Wei Chou, Po-Chih Huang, Ying-Chieh Lin, Ming Jiea Lyu

**Classification :** 35Q35, 35L67, 85A20, 90B20, 35Q20

### **Minisymposium Program :**

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01532 (1/2) : 1C @G704

## [01972] Global BV solution and relaxation limit for Greenberg-Klar-Rascle model

**Author(s) :** Ying-Chieh Lin (National University of Kaohsiung)Shih-Wei Chou (Soochow University)John M. Hong (National Central University)Hsin-Yi Lee (National Cheng Kung University)

**Abstract :** In this talk, we consider the Greenberg-Klar-Rascle multi-lane traffic flow model. This model is a relaxation system with the equilibrium state that is a discontinuous function of the car density. We study the existence of global entropy solutions and the relaxation limit for the GKR model. To construct the approximate solutions, we find two sequences of invariant regions under some suitable condition of initial data. As the relaxation time approaches 0, we prove that the limit of the entropy solutions for the GKR model is a weak solution of its equilibrium equation. It is interesting that the equilibrium equation is a scalar conservation law with discontinuous flux.

## [02450] Global Transonic Solutions of Compressible Euler-Poisson Equations in Semiconductors

**Author(s) :** Shih-Wei Chou (Soochow University)Chia-Chieh Jay Chu (National Tsing Hua University)John M. Hong (National Central University)

**Abstract :** In this talk, we consider an initial-boundary value problem of compressible Euler-Poisson equations arising in semiconductors. The equations form a 3-by-3 hyperbolic system of balance laws with the global source. We establish the global existence of the transonic entropy solution by framework of a generalized Glimm scheme. This is a joint work with John Hong and Jay Chu.

## [02456] Finite Speed of Propagation of the Relativistic Landau and Boltzmann Equations

**Author(s)** : Ming Jiea Lyu (Chung Yuan Christian University)Kung Chien Wu (National Cheng Kung University,)Baoyan Sun (Yantai University)

**Abstract** : In this talk, we will study the relativistic Boltzmann and Landau equations in the whole space  $\mathbb{R}^3$  under the closed to equilibrium setting. We recognize the finite speed of propagation of the solution in  $L_{v,p}^\infty L_x^\infty$  and  $L_v^2 L_x^\infty$ .

## [02865] Global Transonic Solutions of Hot-Jupiter Model for exoplanetary atmosphere

**Author(s)** : Po-Chih Huang (Natonal Chung Cheng University)

**Abstract** : The hydrodynamic escape problem (HEP) for Hot Jupiter model, which is characterized by a initial-boundary value problem of Euler equation with exoplanetary gravity, heat, and tidal force cuased by star, is crucial for investigating the evolution of planetary atmospheres. In this paper, the global existence of transonic solutions to the HEP is established using the generalized Glimm method. The new version of Riemann and boundary-Riemann solvers, are provided as building blocks of the generalized Glimm method by inventing the contraction matrices for the homogeneous Riemann or boundary-Riemann solutions. The extended Glimm-Goodman wave interaction estimates are investigated for obtaining a stable scheme and the lower bound of the gas velocity, which matches the physical observation. The limit of approximation solutions serves as an entropy solution of bounded variations. Moreover, the range of the feasible hydrodynamical region is also obtained.

01532 (2/2) : 1D @G704

## [01545] Interplay between controllability and qualitative aspects of stochastic dynamical systems

**Session Time & Room :**

01545 (1/2) : 4D (Aug.24, 15:30-17:10) @A207

01545 (2/2) : 4E (Aug.24, 17:40-19:20) @A207

**Type** : Proposal of Minisymposium

**Abstract** : This minisymposium highlights recent applications of control-theoretic methods in the study of problems arising in mathematical physics and engineering. Special attention is paid to the interplay between deterministic controllability of dynamical systems and qualitative properties of their counterparts driven by stochastic noise. Both, the regulation of dynamical systems via control forces, and the qualitative investigation of randomness in mathematical models, are strongly motivated by real-world applications. The talks will reflect on current challenges concerning finite-dimensional and infinite-dimensional stochastic systems, deterministic control theory, and the synergetic effects that arise when bringing both topics closer together.

**Organizer(s)** : Manuel Rissel, Vahagn Nersesyan

**Classification** : 93B05, 35R60, 60H15

**Minisymposium Program :**

01545 (1/2) : 4D @A207 [Chair: Manuel Rissel]

## [05477] Mixing via controllability

**Format** : Talk at Waseda University

**Author(s)** : Vahagn Nersesyan (NYU Shanghai)

**Abstract** : In this talk, we will review some recent results where controllability is used to derive mixing for PDEs perturbed by bounded noise.

## [05602] Multi-bubble blow-ups and multi-solitons to focusing (stochastic) nonlinear Schrödinger equations

**Format :** Talk at Waseda University

**Author(s) :** Deng Zhang (Shanghai Jiao Tong University)

**Abstract :** In this talk we mainly review the recent results on multi-bubble blow-ups and multi-solitons to the focusing (stochastic) nonlinear Schrödinger equations. In the mass-critical case, the construction and conditional uniqueness of multi-bubble Bourgain-Wang type blow-up solutions will be presented, which provide new examples for the mass quantization conjecture. In the deterministic case without noise, this also provides new examples of non-pure multi-solitons (including dispersive part) for the soliton resolution conjecture. Furthermore, the refined uniqueness of pure multi-bubble blow-ups and multi-solitons in the very low asymptotic regime is obtained. At last, in both the mass critical and subcritical cases, the direct construction of stochastic multi-solitons will also be presented, particularly, in the absence of the classical pseudo-conformal symmetry.

## [04445] Controllability results for a class of bilinear degenerate wave equations

**Format :** Talk at Waseda University

**Author(s) :** Piermarco Cannarsa (University of Rome Tor Vergata)Patrick Martinez (Université de Toulouse)Cristina Urbani (University of Rome Tor Vergata & Accademia Nazionale dei Lincei)

**Abstract :** I will present a result of exact controllability along the ground state for a degenerate wave equation by means of a bilinear control. We prove that there exists a threshold time  $T_0$  such that: for  $T > T_0$  (and  $T = T_0$  and strong degeneracy) a classical controllability result can be achieved; for  $T <$

## [02831] Small-time approximate controllability for nonlinear Schrödinger equations via bilinear controls

**Format :** Talk at Waseda University

**Author(s) :** Alessandro Duca (Centre Inria Nancy - Grand Est)

**Abstract :** Consider the nonlinear Schrödinger equation (NLS) on a torus of arbitrary dimension in presence of an external potential field whose time-dependent amplitude plays the role of control. We ensure the approximate controllability between eigenstates in arbitrarily small time with respect to the  $L^2$ -norm. We use specific saturation properties to develop a multiplicative version of the geometric approach introduced for additive controls by Agrachev and Sarychev.

01545 (2/2) : 4E @A207 [Chair: Manuel Rissel]

## [03022] Small-time control of bilinear PDEs via infinite-dimensional Lie brackets

**Format :** Online Talk on Zoom

**Author(s) :** Eugenio Pozzoli (Università di Bari)

**Abstract :** We consider PDEs with multiplicative control terms, such as Schrödinger, heat and wave equations. Following a bilinear control strategy recently introduced by Duca and Nersesyan, that is a small-time asymptotic of conjugated dynamics, we investigate some approximate controllability properties of these systems, which hold in arbitrarily small times. We moreover comment on the relation between the controllability properties of the systems and the Lie brackets (a.k.a. commutators) of the operators that generate the dynamics.

## [01547] Optimization in BV and Measure Spaces: Theory and Algorithms

**Session Time & Room :**

01547 (1/3) : 1C (Aug.21, 13:20-15:00) @F402

01547 (2/3) : 1D (Aug.21, 15:30-17:10) @F402

01547 (3/3) : 1E (Aug.21, 17:40-19:20) @F402

**Type :** Proposal of Minisymposium**Abstract :** We consider optimization problems that are posed in the space of Radon measures as well as the space of functions of bounded variation. We present recent theoretical advances, in particular with respect to optimization problems that involve integrality conditions on the distributed optimization variables. These include approximation results in function space that are based on Gamma-convergence, optimality conditions, and consistent discretization schemes. Moreover, the presentations also include recent algorithmic convergence analysis and discrete and stochastic algorithms that allow for efficient solutions of the arising subproblems.**Organizer(s) :** Christian Meyer, Paul Manns**Classification :** 49K30, 49J30, 49N60, 65K10, 90C27**Minisymposium Program :**

01547 (1/3) : 1C @F402 [Chair: Paul Manns]

**[02974] Proximal methods for point source localisation****Format :** Talk at Waseda University**Author(s) :** Tuomo Valkonen (Escuela Politécnica Nacional & University of Helsinki)**Abstract :** Point source localisation is generally modelled as a Lasso-type problem on measures. However, optimisation methods in such non-Hilbert spaces are not yet very well understood. Most numerical algorithms are based on the Frank-Wolfe conditional gradient method. We develop extensions of proximal-type methods to spaces of measures. This includes forward-backward splitting, its inertial version, and primal-dual proximal splitting. Their convergence proofs follow standard patterns. We demonstrate their numerical efficacy.**[04816] Nonsmooth minimization in Banach spaces meets sparse dictionary learning****Format :** Talk at Waseda University**Author(s) :** Daniel Walter (Humboldt Universität zu Berlin)**Abstract :** We propose a novel method for problems involving nonsmooth regularization terms over infinite dimensional function spaces. It resembles a dictionary learning algorithm which updates a dictionary  $\mathcal{A}_k$  of extremal points of the unit ball of the regularizer and of a sparse representation of the iterate  $u_k$  in its conic hull. Imposing additional assumptions on the dual variables, its asymptotic linear convergence is shown.**[04270]  $L^q$ -quasinorm sparse optimal control problems with controls in BV functions****Format :** Talk at Waseda University**Author(s) :** Pedro Martín Merino (Escuela Politécnica Nacional)**Abstract :** We consider an elliptic optimal control of elliptic linear partial differential equations that involves a nonconvex regularization in terms of the  $L^q$  quasi-norm (with  $q$  in  $(0, 1)$ ) together with a TV penalization in the cost function, given by:

$$\mathcal{F}(y, u) = \frac{1}{2} \|y - y_d\|_{L^2(\Omega)}^2 + \frac{\alpha}{2} \|u\|_{L^2(\Omega)}^2 + \beta \int_{\Omega} |u|^q dx + \gamma \int_{\Omega} |Du|,$$

where  $u$  is control and  $y$  are the control and state variables, respectively.

When  $\gamma = 0$ , the classical direct method fails to argue the existence of solutions due to the lack of lower semicontinuity of  $\mathcal{F}$ . However, given the topological properties of  $BV(\Omega)$  and the continuity of the  $L^q$ -quasinorm in  $L^1(\Omega)$ , the existence of solutions can be obtained for controls in  $BV(\Omega)$ . In this talk, we address the optimality conditions for this problem and a numerical approach for its numerical solution based on primal-dual splitting methods.

**[04282] Robust Optimal Experimental Design for Bayesian Inverse Problems****Format :** Talk at Waseda University**Author(s) :** Ahmed Attia (Argonne National Laboratory) Todd Munson (Argonne National Laboratory) Sven Leyffer (Argonne National Laboratory)**Abstract :** An optimal design is defined as the one that maximizes a predefined utility function which is

part\_2

formulated in terms of the elements of an inverse problem. An example being optimal sensor placement for parameter identification. This formulation generally overlooks misspecification of the elements of the inverse problem such as the prior or the measurement uncertainties. In this talk, we present efficient recipes for designing optimal experimental design schemes, for Bayesian inverse problems, such that the optimal design is robust with respect to misspecification of elements of the inverse problem.

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01547 (2/3) : 1D @F402 [Chair: Paul Manns]

## [03634] Opial property in Wasserstein spaces and applications

**Format :** Talk at Waseda University

**Author(s) :** Emanuele Naldi (TU Braunschweig)

**Abstract :** The Opial property is a metric characterization of weak convergence for a suitable class of Banach spaces. It plays an important role in the study of weak convergence of iterates of mappings and of the asymptotic behavior of nets satisfying some metric properties. Since it involves only metric quantities, it is possible to define this property also in metric spaces provided with a suitable notion of weak convergence. This is the case for spaces of probability measures endowed with the Kantorovich-Rubinstein-Wasserstein metric deriving by optimal transport. In particular, in this talk, we present an Opial property in the Wasserstein space of Borel probability measures with finite quadratic moment on a separable Hilbert space. We present applications of this property to convergence of Wasserstein gradient flows of lower semicontinuous and geodesically convex functionals defined on the space of probability measures. We show further application to convergence of sequences generated by the proximal point algorithm and a proximal gradient algorithm when the functional satisfy some additional hypothesis. We conclude with one last application of the property to convergence to a fixed point for iterations of a non-expansive map defined on a weakly closed set.

## [03671] An Optimal Transport-based approach to Total-Variation regularization for the Diffusion MRI problem

**Format :** Talk at Waseda University

**Author(s) :** Rodolfo Asereto (University of Graz)Kristian Bredies (University of Graz)Marion I. Menzel (GE Global Research, Munich)Emanuele Naldi (TU Braunschweig)Claudio Mayrink Verdun (TU München)

**Abstract :** Diffusion Magnetic Resonance Imaging (dMRI) is a non-invasive imaging technique that draws structural information from the interaction between water molecules and biological tissues. Common ways of tackling the derived inverse problem include, among others, Diffusion Tensor Imaging (DTI), High Angular Resolution Diffusion Imaging (HARDI) and Diffusion Spectrum Imaging (DSI). However, these methods are structurally unable to recover the full diffusion distribution, only providing partial information about particle displacement. In our work, we introduce a Total-Variation (TV) regularization defined from an optimal transport perspective using 1-Wasserstein distances. Such a formulation produces a variational problem that can be handled by well-known algorithms enjoying good convergence properties, such as the primal-dual proximal method by Chambolle and Pock. It allows for the reconstruction of the complete diffusion spectrum from measured undersampled k/q space data.

## [04791] A minimization problem in the space of bounded deformations arising in visco-plastic fluid flows

**Format :** Talk at Waseda University

**Author(s) :** Lukas Holbach (Johannes Gutenberg University Mainz)Christian Meyer (TU Dortmund)Georg Stadler (New York University)

**Abstract :** Plasticity and material failure play an important role in Earth's plate motion. These phenomena are commonly modeled by incompressible Stokes flows with visco-plastic rheologies. Weak solutions of these nonlinear equations can be characterized as minimizers of a convex energy functional. While the solution is unique and lies in  $H^1$  if a lower-bound regularization on the viscosity is employed, the problem becomes singular without regularization and the solution must be sought in the space of bounded deformations (BD).

We present an existence result in BD and show that the regularized solutions converge to a solution of the singular problem with respect to a suitable topology when the regularization parameter tends to zero.

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01547 (3/3) : 1E @F402 [Chair: Paul Manns]

## [03554] Solving Discrete Subproblems of a Trust-Region Algorithm for MIOCP

**Format :** Talk at Waseda University

**Author(s) :** Marvin Severitt (TU Dortmund University)Paul Manns (TU Dortmund University)

**Abstract :** We consider a trust-region algorithm for the solution of control problems, where the control input is an integer-valued function and is regularized with a total variation term in the objective. A class of integer linear programs arises as discretizations of the trust-region subproblems. We discuss how, in the one-dimensional case, the discretized subproblems can be solved with a graph-based approach and how the information obtained can be used for the two-dimensional case.

## [03555] Regularization and outer approximation for optimal control problems in BV

**Format :** Talk at Waseda University

**Author(s) :** Annika Müller (TU Dortmund University)Christian Meyer (TU Dortmund University)

**Abstract :** We consider optimal control problems with a constraint on the TV-seminorm of the control. We replace the TV-seminorm by a regularized version and solve the resulting optimization problems with an outer approximation algorithm. We prove convergence of the algorithm to the globally optimal solutions, which in turn converge to the optimal solution to the original problem as the regularization parameter vanishes.

## [03256] On integer optimal control problems with total variation regularization

**Format :** Talk at Waseda University

**Author(s) :** Jonas Marko (BTU Cottbus-Senftenberg)Gerd Wachsmuth (BTU Cottbus-Senftenberg)

**Abstract :** We investigate integer optimal control problems of the form

$$\text{Minimize } F(u) + \beta \text{TV}(u) \quad \text{s.t. } u(t) \in \{\nu_1, \dots, \nu_d\} \subset \mathbb{Z} \text{ for a.a. } t \in (0, T)$$

with  $\beta > 0$ . The contribution  $F$  is assumed to be differentiable and could e.g. realize the tracking of the state given by an ODE or PDE dependent on  $u$ .

We show local optimality conditions of first and second order as well as non-local optimality conditions. Also, we will calculate numerical solutions exemplary on two specific control problems.

## [04006] Non-uniform Grid Refinement for the Combinatorial Integral Approximation

**Format :** Talk at Waseda University

**Author(s) :** Christoph Hansknecht (TU Clausthal)Paul Manns (TU Dortmund University)

**Abstract :** We examine mixed-integer optimal control problems (MIOCP) with a discrete-valued control variable distributed on a two-dimensional domain.

We compute integral controls by rounding fractional ones according to the combinatorial integral approximation (CIA) framework with switching costs modeling total variation. The rounding problem becomes computationally challenging in two dimensions, leading us to examine both heuristic and exact solution approaches, reducing the number of problem variables based on non-uniform grid refinements.

## [01605] Recent advances in computational methods for kinetic and hyperbolic equations

**Session Time & Room :**

01605 (1/2) : 5B (Aug.25, 10:40-12:20) @E702

01605 (2/2) : 5C (Aug.25, 13:20-15:00) @E702

**Type :** Proposal of Minisymposium

**Abstract :** In recent years, there have been significant advances in computational algorithms for kinetic and hyperbolic equations. New methods have been designed that can achieve efficient simulations while preserving key structures of the underlying solutions. This minisymposium will bring experts in this area to present some key advances, including numerical methods and model reduction for wave equations and kinetic equations. Novel schemes and their properties will be discussed with applications in electromagnetic waves, plasma simulations and applications in gas dynamics and nuclear engineering.

**Organizer(s) :** Yingda Cheng

**Classification :** 65M22

**Minisymposium Program :**

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01605 (1/2) : 5B @E702 [Chair: Yingda Cheng]

### [03143] A Natural Model Reduction Framework for Kinetic Equations

**Format :** Talk at Waseda University

**Author(s) :** Ruo Li (Peking University)

**Abstract :** To investigate a kinetic equation with prescribed low dimensional input data set, the solutions provided by the equation has to be confined in a low dimensional manifold. We propose in this article a natural framework for the model reduction of the kinetic equation with such the setup that an approximate solution manifold with finite dimension is available. The method results in a symmetric hyperbolic system automatically with natural assumptions. As the applications of the framework, we present some interesting cases, some of which gives brand-new models with elegant features. A few essential factors, including conservative quantities and entropy increasing, can be discussed in terms of the properties of the approximate the solution manifold.

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01605 (2/2) : 5C @E702

## [01622] Mathematics for Prediction and Control of Complex Systems

**Session Time & Room :**

01622 (1/3) : 3D (Aug.23, 15:30-17:10) @D408

01622 (2/3) : 3E (Aug.23, 17:40-19:20) @D408

01622 (3/3) : 4C (Aug.24, 13:20-15:00) @D408

**Type :** Proposal of Minisymposium

**Abstract :** Weather is a good example of large-scale chaotic complex systems, with a strong sensitivity to initial conditions tied to the intrinsic limit to predictability. The sensitivity suggests effective control in which small modifications to the atmospheric conditions grow rapidly and result in big changes. Weather predictability has been studied extensively in the past decades, and prediction skills have been improving. With accurate weather prediction, we are now ready to study weather controllability. This mini-symposium consists of solicited presentations about the mathematics behind the predictability and controllability of complex systems such as weather and other problems.

**Organizer(s) :** Takemasa Miyoshi, Sebastian Reich, Takashi Sakajo, Kohei Takatama

**Classification :** 86A08, 34H10, 93B05, 93E11, 76F70

**Minisymposium Program :**

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01622 (1/3) : 3D @D408 [Chair: Takemasa Miyoshi]

### [02251] Sequential data assimilation and data driven control

**Format :** Online Talk on Zoom

**Author(s) :** Sebastian Reich (University of Potsdam)

**Abstract :** Sequential data assimilation can be considered a coupling of measure problem which can be tackled using optimal transport or Schroedinger bridges. In this talk, we will present an approximate bridging approach

which leads to a data-driven term being added to the underlying model dynamics. The added control term is of mean-field type and can be implemented easily within a Monte Carlo context. The control term is also closely related to continuous time ensemble Kalman-Bucy filter formulations. One can extend the proposed controlled DA approach to cost functions other than those derived from the data likelihood.

## [02790] Data-driven Reconstruction of Partially Observed Dynamical Systems

**Format :** Talk at Waseda University

**Author(s) :** Pierre Tandeo (IMT Atlantique)Pierre Ailliot (Univ. Brest)Florian Sévellec (CNRS)

**Abstract :** The goal of this work is to obtain predictions of a partially observed dynamical system, without knowing the model equations. To account to those strong assumptions, a combination of machine learning and data assimilation techniques is proposed with the introduction of latent variables. We find that the latent variables inferred by the procedure are related to the successive derivatives of the observed components of the dynamical system.

## [02800] Sensor selection by greedy method for linear dynamical systems

**Format :** Talk at Waseda University

**Author(s) :** Shun Takahashi (Tokai University)Kumi Nakai (National Institute of Advanced Industrial Science and Technology )Takayuki Nagata (Tohoku University)Keigo Yamada (Tohoku University)Yasuo Sasaki (Tohoku University)Yuji Saito (Tohoku University)Taku Nonomura (Tohoku University)

**Abstract :** Sensor optimization using a greedy method based on the snapshot-to-snapshot Fisher information matrix, observability Gramian, and Kalman filter indices in linear time-invariant systems is discussed. The objective functions and computational times are compared for the resulting sensor sets with a background of application to sensor selection in large systems.

## [02804] Fast Linear-regression-based Sensor Selection and its Applications

**Format :** Talk at Waseda University

**Author(s) :** Yasuo Sasaki (Tohoku University)Yuji Saito (Tohoku University)Takayuki Nagata (Tohoku University)Keigo Yamada (Tohoku University)Taku Nonomura (Tohoku University)

**Abstract :** We consider a ridge-regression-based sensor selection problem in which sensors are selected so that dependent variables can be estimated as easily as possible. For this problem, a fast greedy algorithm is derived by means of one-rank update law of covariance matrices. To verify the effectiveness of this greedy algorithm, it is applied to sensor selection for estimation of the sea surface temperature and for optimal feedback control of flow around a circular cylinder.

01622 (2/3) : 3E @D408 [Chair: Sebastian Reich]

## [02789] Identifying Coherent Structures within Turbulent Flows over Roughness Obstacles

**Format :** Talk at Waseda University

**Author(s) :** Tetsuya Takemi (Kyoto University)

**Abstract :** Large-eddy simulations for turbulent flows over roughness obstacles are conducted to investigate the characteristics of coherent structures within turbulent flows for a possible application for controlling flow structures in urban districts. Idealized and realistic urban districts are examined as rough surfaces. Turbulence and dispersion properties associated with coherent structures are demonstrated. Understanding such properties will lead to identify an approach to control flows within urban districts.

## [02825] Quantifying Weather Controllability and Mitigatable Flood Damage Based on Ensemble Weather Forecast

**Format :** Talk at Waseda University

**Author(s) :** Shunji Kotsuki (Chiba University)

**Abstract :** For realizing a weather-controlled society, we need to discuss the way to maximize the effect of manipulations to the atmosphere. For that purpose, this project aims at developing methods that quantify weather controllability and mitigatable flood damage based on ensemble weather forecasts. To quantify weather controllability, this project investigates meteorological landscapes that separate disaster and non-disaster regimes

which may be controllable with small manipulations. We also estimate economic damages under non-controlled/controlled scenarios, in order to quantify avoidable damage by weather control.

We have started illustrating directed graphs as the first step in understanding the meteorological landscape. Typhoon Papiroon in 2018 was used for the case study. Singular value decomposition (SVD) is employed for Japan Meteorological Agency's operational meso-scale ensemble prediction data to extract principle components of atmospheric states, followed by a clustering using density-based spatial clustering of applications with noise known as DBSCAN. The illustrated graph succeeded in detecting separated two clusters that correspond to faster and slower movements of predicted Parapiroon. The developed algorithm is currently applied to other disastrous events as well as further investigations on non-linear data compression methods beyond SVD. This presentation includes the most recent achievements up to the time of the conference.

## **[02885] Ensemble sensitivity and its potential applications in weather control**

**Author(s)** : Le Duc (University of Tokyo)Yohei Sawada (University of Tokyo)

**Abstract** : Ensemble sensitivity has been proved to be a very useful sensitivity measure in practice. In this study, we show the relevance of ensemble sensitivity in another important problem. We have proved that changes of the forecast response are maximized along the direction of the vector consisting of ensemble sensitivities which forms the most sensitive perturbation. We will demonstrate how the new understanding on ensemble sensitivities can qualitatively give potential solutions for weather control.

## **[02518] Chaos implies effective controllability of extreme weather**

**Format** : Talk at Waseda University

**Author(s)** : Takemasa Miyoshi (RIKEN)Qiwen Sun (RIKEN)Koji Terasaki (RIKEN)Yasumitsu Maejima (RIKEN)

**Abstract** : Since the weather system is chaotic, and even more so for storms, small differences generally lead to big differences, particularly for high-impact weather events. This presentation will summarize the concept and methodology of Control Simulation Experiment (CSE) with some proof-of-concept demonstrations with toy models and realistic Numerical Weather Prediction (NWP) models. This is an attempt to a potential paradigm change of NWP research from decades of predictability to the new era of controllability.

01622 (3/3) : 4C @D408 [Chair: Takashi Sakajo]

## **[02814] Noise Calibration for the Stochastic Rotating Shallow Water Equations**

**Format** : Talk at Waseda University

**Author(s)** : Alexander Lobbe (Imperial College London)Oana Lang (Imperial College London)Dan Crisan (Imperial College London)Peter Jan van Leeuwen (Colorado State University)Roland Potthast (Deutscher Wetterdienst DWD)

**Abstract** : We introduce a new method of noise calibration of the Stochastic Rotating Shallow Water (SRSW) model which is rigorously derived from a model reduction technique. The method is generic and can be applied to arbitrary stochastic models. In the (SRSW) case, we calibrate the noise by using the pressure variable of the model, as this is an observable easily obtainable in practical application.

## **[03049] Machine learning-based estimation of state-dependent forecast uncertainty**

**Format** : Talk at Waseda University

**Author(s)** : Juan Jose Ruiz (University of Buenos Aires)Maximiliano Sacco (National Meteorological Service of Argentina)Manuel Pulido (Universidad Nacional del Nordeste)Pierre Tandeo (IMT Atlantique)

**Abstract** : Quantifying forecast uncertainty is a key aspect of state-of-the-art numerical weather prediction and data assimilation systems. State dependent uncertainty quantification in numerical weather prediction is a computation intensive task which has been performed using different approaches such as monte carlo sampling (ej. ensemble Kalman filter) and variational approaches (ej. adjoint based model sensitivity). Machine learning techniques consist of trainable statistical models that can represent complex functional dependencies among different groups of variables given a large enough dataset. In this talk we will describe the use of a machine learning approach based on neural networks for the estimation of forecast uncertainty. In particular, we will discuss the estimation of the forecast error covariance matrix, which is at the center of probabilistic forecasting and data assimilation systems. In addition, we will present a hybrid data assimilation method that combines the

optimal interpolation technique and a convolutional neural network to estimate the state dependent forecast error covariance matrix.

### **[03126] Observability of continuous-time Markov model and filter stability**

**Format :** Talk at Waseda University

**Author(s) :** JIN WON KIM (University of Potsdam)

**Abstract :** In control theory, estimation and control are considered as dual problems. A fundamental relationship is the duality between controllability and observability, and it extends to Kalman filter and a linear quadratic control problem. Our contribution is to extend the duality to nonlinear models. I will review the classical duality and present the dual optimal control problem. The dual formulation is used to analyze the stability of the nonlinear filter, similar to the linear Gaussian case.

### **[03024] On random feature maps in prediction**

**Format :** Talk at Waseda University

**Author(s) :** Nicholas Cranch (University of Sydney)Georg A. Gottwald (University of Sydney)Sebastian Reich (University of Potsdam)

**Abstract :** Random feature maps (RFs) can be viewed as a single hidden layer network in which the weights of the hidden layer are fixed. We show how the choice of the internal weights effects performance and generalisation. We propose how to best choose the internal weights. We show that RFs allow for sequential learning when combined with data assimilation, and can be used to learn subgrid-scale parametrizations and to detect critical transitions.

## **[01661] Recent Development on the Methods and Applications of Complex PDE systems**

**Session Time & Room :**

01661 (1/2) : 2D (Aug.22, 15:30-17:10) @E606

01661 (2/2) : 2E (Aug.22, 17:40-19:20) @E606

**Type :** Proposal of Minisymposium

**Abstract :** Complex partial differential equations have been widely applied to different areas to understand the spatiotemporal dynamics of multiple interactive components, such as reaction-diffusion equations for modeling diffusive molecules in biology, Navier-Stokes equations for modeling fluid dynamics. Traditional numerical approaches may fail when applied to PDE models in applications due to specific features of application problems. In this minisymposium, we will focus on the recent development of new numerical approaches and applications of different PDE systems. The goal of this session is to bring together researchers in numerical PDEs and mathematical models to exchange ideas and explore collaborations.

**Organizer(s) :** Weitao Chen, Huijing Du, Yuan Liu

**Classification :** 65Z05, 65M99, 65-04, 92-08, 92-10

**Minisymposium Program :**

01661 (1/2) : 2D @E606 [Chair: Huijing Du]

### **[04291] A learned conservative semi-Lagrangian finite volume scheme for transport simulations**

**Format :** Talk at Waseda University

**Author(s) :** Wei Guo (Texas Tech University)Yongsheng Chen (Zhejiang University)Xinghui Zhong (Zhejiang University)

**Abstract :** Semi-Lagrangian (SL) schemes are known as a major numerical tool for solving transport equations with many. In this talk, we introduce a novel machine learning-assisted approach to accelerate the conventional SL finite volume schemes. The proposed scheme avoids the expensive tracking of upstream cells but attempts to learn

the SL discretization from the data by incorporating specific inductive biases in the neural network, significantly simplifying the algorithm implementation and leading to improved efficiency.

## [03990] A new type of simplified inverse Lax-Wendroff boundary treatment for hyperbolic conservation laws

**Format :** Talk at Waseda University

**Author(s) :** Shihao Liu (University of Science and Technology of China)Tingting Li (Henan University)Ziqiang Cheng (Hefei University of Technology)Yan Jiang (University of Science and Technology of China)Chi-Wang Shu (Brown University)Mengping Zhang (University of Science and Technology of China)

**Abstract :** In this talk, we will introduce a new kind of high order inverse Lax-Wendroff (ILW) boundary treatment for solving hyperbolic conservation laws with finite difference method on a Cartesian mesh, in which both scalar equations and systems are considered. This new ILW method decomposes the construction of ghost points into two steps: interpolation and extrapolation. At first, we approximate some special points value through interpolation polynomial given the interior points near boundary. Then, we will construct a Hermite extrapolation polynomial based on those special point values and spatial derivatives at boundary obtained through ILW process. This extrapolation polynomial will give us the approximation of the the ghost points value. Eigenvalue analysis shows that the new method can improve the computational efficiency on the premise of maintaining accuracy and stability. Numerical tests for one- and two-dimensional problems indicate that our method has high order accuracy for smooth solutions and non-oscillatory property for shock solution near boundary.

## [02713] Transmission Dynamics of Tuberculosis with Age-specific Disease Progression

**Format :** Talk at Waseda University

**Author(s) :** Wing-Cheong Lo (City University of Hong Kong)

**Abstract :** In this talk, we develop a system of delay partial differential equations to model tuberculosis transmission in a heterogeneous population. The system considers demographic structure coupling with the continuous development of the disease stage. We determine the basic reproduction number and several numerical simulations are used to investigate the influence of various progression rates on tuberculosis dynamics. This is joint work with Yu Mu, Tsz-Lik Chan, and Hsiang-Yu Yuan.

## [02985] Extended-release Pre-Exposure Prophylaxis and Drug Resistant HIV

**Format :** Talk at Waseda University

**Author(s) :** Yanping Ma (Loyola Marymount University)Yeona Kang (Howard University)Angelica Davenport (Florida State University)Jennifer Aduamah (University of Delaware)Kathryn Link (Pfizer)Katharine Gurski (Howard University)

**Abstract :** We present a within-host, mechanistic Differential Equation model of the HIV latency and infection cycle in CD4+ T-cells to investigate drug-resistant mutations. We develop a pharmacokinetic/pharmacodynamic model for long-acting cabotegravir (CAB-LA, injectable PrEP) to relate the inhibitory drug response to the drug concentration in plasma and rectal, cervical, and vaginal fluids and tissue. And we will report some of our important findings in the talk.

01661 (2/2) : 2E @E606 [Chair: Weitao Chen]

## [04493] A Level-Set Framework for Implicit Solvation

**Format :** Talk at Waseda University

**Author(s) :** Li-Tien Cheng (UC San Diego)

**Abstract :** Implicit solvation involves the study of the effects solute atoms have on a surrounding solvent, which can be particularly important in, for example, the process of protein docking. An implicit treatment of the solvent gives rise to an interface between solute and solvent. We introduce a level-set framework applied to a variational free-energy setup for constructing such an interface, and consider efficient and accurate solvers in the presence of curvature, electrostatic, and mechanical effects.

## [04909] Adaptive ANOVA and reduced basis methods to anisotropic stochastic PDEs

**Format :** Talk at Waseda University

**Author(s) :** Heyrim Cho (University of California Riverside)Bedřich Sousedík (University of Maryland, Baltimore County)Howard Elman (University of Maryland, College Park)

**Abstract :** The combination of reduced basis and collocation methods enables efficient and accurate evaluation of the solutions to parameterized PDEs. We study the stochastic collocation methods that can be combined with reduced basis methods to solve high-dimensional parameterized stochastic PDEs. We also propose an adaptive algorithm using a probabilistic collocation method (PCM) and ANOVA decomposition. This procedure involves two stages. First, the method employs an ANOVA decomposition to identify the effective dimensions, i.e., subspaces of the parameter space in which the contributions to the solution are larger, and sort the reduced basis solution in a descending order of error. Then, the adaptive search refines the parametric space by increasing the order of polynomials until the algorithm is terminated by a saturation constraint. We demonstrate the effectiveness of the proposed algorithm for solving a stationary stochastic convection-diffusion equation, a benchmark problem chosen because solutions contain steep boundary layers and anisotropic features. We also solve the Stokes-Brinkman equations that model fluid flow in highly heterogeneous porous media.

## [04915] Theoretical Principles of Enhancer-Promoter Communication in Gene Expression

**Format :** Talk at Waseda University

**Author(s) :** Jiajun Zhang (Sun Yat-sen University)

**Abstract :** Recent experimental evidence strongly supports that long-range enhancer-promoter interactions have important influences on gene-expression dynamics, but it is unclear how the interaction information is translated into gene expression over time. To address this challenge, we develop a general theoretical framework that integrates chromatin dynamics, enhancer-promoter communication, and gene-state switching to study gene expression. Our model and results provide quantitative insight into both spatiotemporal gene-expression determinants and cellular fates during development.

# [01671] Financial Modeling

**Session Time & Room :**

01671 (1/2) : 2D (Aug.22, 15:30-17:10) @D502

01671 (2/2) : 2E (Aug.22, 17:40-19:20) @D502

**Type :** Proposal of Minisymposium

**Abstract :** Financial activities are principally based on a variety of models, which have been modified over times according to the change of financial situation as well as the change of financial regulation. The corresponding stochastic mathematical models are also adjusted. In recent years, disaster risk financing and insurance strategy are of importance. In this minisymposium, we present researches of various aspects of financial modeling, from basic theory to real world problems.

**Organizer(s) :** Naoyuki Ishimura, Rita Helbra Tenrini

**Classification :** 91-10, 91-08

**Minisymposium Program :**

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01671 (1/2) : 2D @D502 [Chair: Naoyuki Ishimura]

## [05403] Insurance design for the loss of epidemic outbreaks involving the Cramer -Lundberg model

**Format :** Talk at Waseda University

**Author(s) :** Naoyuki Ishimura (Chuo University)Chenwei Sun (Chuo University)Koichiro Takaoka (Chuo University)

**Abstract :** We consider the insurance design for the loss of epidemic outbreaks such as COVID-19. The new point of our model is to involve the Cramer-Lundberg process in the risk theory. Utilizing the standard time-discrete SIR

model, we propose how to compute the insurance coverage due to the damage of epidemic bursts. The comparison between our theory and the empirical study employing the daily data of Tokyo area will be also discussed.

## [02749] Micro-foundations of some financial models with bubbles

**Format :** Talk at Waseda University

**Author(s) :** Naohiro Yoshida (Keio University)

**Abstract :** This presentation will discuss the micro-foundation of some financial models with bubbles.

The micro-foundation discussed is the excess demand model. In other words, the amount of demand for and supply of a security by each investor in the market are formulated, and the price of the security is determined so that they satisfy the market-clearing condition.

The main objective of this presentation is to propose some excess demand models of financial models with bubbles. We will discuss what characteristics of investor's demand and supply cause bubbles.

## [02787] An Ito-Wentzell Formula for SDE Conditional Measure Flows

**Format :** Talk at Waseda University

**Author(s) :** Nizar Touzi (CMAP, Ecole Polytechnique) Assil Fadle (CMAP, Ecole Polytechnique)

**Abstract :** We provide general Ito and Ito-Wentzell formulas for functions of conditional measure flows of continuous semimartingales, using functional linear derivatives and standard stochastic analysis results. We provide applications for mean field optimal control and mean field optimal stopping with common noise.

## [04500] A Generalized Cramér-Lundberg Model Driven by Mixed Poisson Processes

**Format :** Talk at Waseda University

**Author(s) :** Masashi Tomita (Meiji Yasuda Life Insurance Company) Koichiro Takaoka (Chuo University) Motokazu Ishizaka (Chuo University)

**Abstract :** We propose a generalized Cramér-Lundberg model of the risk theory of non-life insurance and discuss several mathematical properties including the ruin probability. Our model is an extension of that of Dubey (1977) to the case of multiple insureds, where the counting process is a mixed Poisson process and the continuously varying premium rate is determined by a Bayesian rule on the number of claims.

01671 (2/2) : 2E @D502

## [01672] High accuracy compact methods for partial differential equations

**Session Time & Room :**

01672 (1/2) : 3C (Aug.23, 13:20-15:00) @E704

01672 (2/2) : 3D (Aug.23, 15:30-17:10) @E704

**Type :** Proposal of Minisymposium

**Abstract :** This minisymposium brings together researchers developing high accuracy compact finite difference schemes for the solution of a variety of partial differential equations. One of the aims of this minisymposium is to examine the progress made on the solution of a variety of fluid flow problems.

**Organizer(s) :** Murli M Gupta

**Classification :** 65N06, 65N12, 76D05, 65N30

**Minisymposium Program :**

01672 (1/2) : 3C @E704 [Chair: Murli M. Gupta]

## [05366] Spectral Element Method for Parabolic Problems with Corner Singularities

**Format :** Talk at Waseda University

**Author(s) :** Sanuwar Ahmed Choudhury (National Institute of Technology Silchar Assam India)Pankaj Biswas (National Institute of Technology Silchar Assam India)

**Abstract :** In many engineering applications, reconstruction of temperature generated from incomplete data causes corner singularities. In such cases, a solution of parabolic initial-boundary-value-problems(IBVP) on nonsmooth-domains is required. Spectral-element methods give exponential accuracy for smooth solutions. Generating geometric meshes at the neighborhood of the corners on the space-domain a parallel least-squares-spectral-element-method using MPI is presented here to resolve the singularities. Numerical scheme has been developed in the frame-work of Sobolev spaces and examples are presented to validate the estimates.

01672 (2/2) : 3D @E704 [Chair: Jiten C. Kalita]

## [01681] Recent advances in numerical methods for partial differential equations

**Session Time & Room :**

01681 (1/3) : 1C (Aug.21, 13:20-15:00) @E711

01681 (2/3) : 1D (Aug.21, 15:30-17:10) @E711

01681 (3/3) : 1E (Aug.21, 17:40-19:20) @E711

**Type :** Proposal of Minisymposium

**Abstract :** Partial differential equations are a family of powerful mathematical tools to model the physical world. In many practical situations, it is generally very difficult to obtain their analytical solutions, and thus numerical methods become critical for simulation. This mini-symposium aims to bring together scholars to discuss the recent advances and innovative techniques in this field including finite element exterior calculus, physics-preserving schemes, polytopal meshes and high-order methods. The mini-symposium will also deal with the applications onto electromagnetism, fluid dynamics and interface problems.

**Organizer(s) :** Long Chen, Ruchi Guo, Liuqiang Zhong

**Classification :** 65N30, 65M60, 65N50, 65N55

**Minisymposium Program :**

01681 (1/3) : 1C @E711 [Chair: Long Chen]

## [03945] Geometrical degrees of freedom for high order Whitney forms

**Format :** Talk at Waseda University

**Author(s) :** Ana María Alonso Rodríguez (University of Trento)Francesca Rapetti (Université Côte d'Azur)Ludovico Bruni Bruno (Università dell'Insubria)

**Abstract :** Finite element spaces extending Whitney forms to higher polynomial degrees are widely used for discretizing partial differential equations in electromagnetism, fluid dynamics or elasticity, and different degrees of freedom (dofs) can be considered for interpolation. In particular the so-called weights preserve the meaning of the natural degrees of freedom associated with Whitney forms as circulation, fluxes or densities since they are the integrals of a k-form on k-chains. Weights are a generalization of the evaluations of a scalar function at a set of nodes in view of its reconstruction on multivariate polynomial bases and allows to extend in a natural way well-known concepts as the Lebesgue constant. We rely on the flexibility of the weights with respect to their geometrical support to reduce the growth of the Lebesgue constant when increasing the degree of the polynomial interpolation of differential k-forms.

## [02919] Energy-preserving Mixed finite element methods for a ferrofluid flow model

**Format :** Talk at Waseda University

**Author(s) :** Yongke Wu (University of Electronic Science and Technology of China)Xiaoping Xie (Sichuan University)

**Abstract :** In this talk, we introduce a class of mixed finite element methods for the ferrofluid flow model proposed by Shliomis [Soviet Physics JETP, 1972]. We show that the energy stability of the weak solutions to the model is preserved exactly for both the semi- and fully discrete finite element solutions. Furthermore, we prove the existence of the discrete solutions and derive optimal error estimates for both the the semi- and fully discrete schemes. Numerical experiments confirm the theoretical results.

## [03132] Immersed CR element methods for the elliptic and Stokes interface problems

**Format :** Talk at Waseda University

**Author(s) :** Haifeng Ji (Nanjing University of Posts and Telecommunications)FENG WANG (NanJing Normal University)Jinru Chen (NanJing Normal University)Zhilin Li (North Carolina State University)

**Abstract :** In this talk, we shall discuss the immersed CR element method for solving the elliptic and Stokes interface problems with piecewise constant coefficients that have jumps across the interface. In the method, the triangulation does not need to fit the interface and the IFE spaces are constructed from the traditional CR element with modifications near the interface according to the interface jump conditions. The stability and the optimal error estimates of the proposed methods are also derived rigorously. The constants in the error estimates are shown to be independent of the interface location relative to the triangulation. Numerical examples are provided to verify the theoretical results.

## [02917] A fast Cartesian grid method for unbounded interface problems with non-homogeneous source terms

**Format :** Talk at Waseda University

**Author(s) :** Jiahe Yang (Shanghai Jiao Tong University)Wenjun Ying (Shanghai Jiao Tong University)

**Abstract :** A Cartesian grid method is presented for interface problems of PDEs with non-homogeneous source terms on unbounded domains. The method adapts a compression-decompression technique and has algorithm complexity of only  $O(n^2 \log n)$  as compared to  $O(n^3)$  by traditional methods. This Cartesian grid method is an extension of the kernel-free boundary integral method, which avoids direct evaluation of singular or nearly singular integrals by reformulating them into solutions of equivalent but much simpler interface problems.

01681 (2/3) : 1D @E711 [Chair: Liuqiang Zhong]

## [04905] Staggered DG methods for elliptic problems on general meshes

**Format :** Talk at Waseda University

**Author(s) :** Eun-Jae Park (Yonsei University)

**Abstract :** In this talk, we present our recent framework on staggered DG methods for elliptic equations on general meshes, which can be flexibly applied to rough grids such as highly distorted meshes.

Adaptive mesh refinement is an attractive tool for general meshes due to their flexibility and simplicity in handling hanging nodes.

We derive a simple residual-type error estimator. Numerical results indicate that optimal convergence can be achieved for both the potential and vector variables, and the singularity can be well-captured by the proposed error estimator. Then, some applications to Darcy-Forchheimer equations, Stokes equations, and linear elasticity equations are considered. This is joint work with Eric Chung, Dohyun Kim, Dong-wook Shin, and Lina Zhao.

## [04160] Accelerated Gradient and Skew-Symmetric Splitting Methods for Monotone Operator Equations

**Format :** Online Talk on Zoom

**Author(s) :** Jingrong Wei (University of California, Irvine) Long Chen (University of California at Irvine)

**Abstract :** A class of monotone operator equations, which can be decomposed into sum of a gradient of a strongly convex function and a linear and skew-symmetric operator, is considered in this work. Based on discretization of the generalized accelerated gradient flow, accelerated gradient and skew-symmetric splitting (AGSS) methods are developed and shown to achieve linear rates with optimal lower iteration complexity when applied to smooth saddle point systems with bilinear coupling.

## [03693] Solve electromagnetic interface problems on unfitted meshes

**Format :** Talk at Waseda University

**Author(s) :** Ruchi Guo (University of California Irvine)

**Abstract :** Electromagnetic interface problems widely appear in a lot of engineering applications, such as electric actuators, invasive detection techniques and integrated circuit , which are typically described by Maxwell equations with discontinuous coefficients. Conventional finite element methods require a body-fitted mesh to solve interface problems, but generating a high-quality mesh for complex interface geometry is usually very expensive. Instead using unfitted mesh finite element methods can circumvent mesh generation procedure, which greatly improve the computational efficiency. However, the low regularity of Maxwell equations makes its computation very sensitive to the conformity of the approximation spaces. This very property poses challenges on unfitted mesh finite element methods, as most of them resort to non-conforming spaces. In this talk, we will present our recent progress including several methods for this topic.

## [03714] Pressure-robust virtual element methods for the Stokes problem on polygonal meshes

**Format :** Talk at Waseda University

**Author(s) :** Gang Wang (Northwestern Polytechnical University)

**Abstract :** In this talk, we shall introduce two pressure-robust virtual element methods for the Stokes problem on polygonal meshes. The standard virtual element scheme involves a pressure contribution in the velocity error. To achieve the pressure-independent velocity approximation, we define an H(div)-conforming velocity reconstruction operator for the velocity test function and propose the modified scheme by employing it in the approximation of right-hand-side source term assembling. In the first method, we apply the H(div)-conforming elements on the polygons and construct a (theoretically) exactly pressure-robust virtual element scheme. Since basis functions of H(div)-conforming elements are not polynomials on general polygons, quadrature errors will affect the exact pressure-robustness in implementation. To solve it, we reconstruct a (theoretically and numerically) exactly pressure-robust virtual element scheme by designing H(div)-conforming element based on the sub-triangulation of polygon and the lowest-order Raviart-Thomas element. We give the error estimates of two methods and also show numerical examples to support our theories.

01681 (3/3) : 1E @E711 [Chair: Ruchi Guo]

## [05142] Arbitrary order DG-DGLM method for hyperbolic systems of multi-dimensional conservation laws

**Format :** Talk at Waseda University

**Author(s) :** Mi-Young Kim (Inha University)

**Abstract :** An arbitrary order discontinuous Galerkin method with Lagrange multiplier in space and time is proposed to approximate the solution to hyperbolic systems of multi-dimensional conservation laws. Weak formulation is derived through the definition of weak divergence. Weak solution on the edge is characterized as the average of the solutions on the elements sharing the edge. Stability of the approximate solution is proved in a broken  $L_2(L_2)$  norm. Error estimates of  $O(h^r + k_n^q)$  with  $P_r(E)$  and  $P_q(J_n)$  elements ( $r, q > 1 + d/2$ ) are then derived in a broken  $L_2(L_2)$  norm, where  $h$  and  $k_n$  are the maximum diameters of the elements and the time step of  $J_n$ , respectively,  $J_n$  is the time interval, and  $d$  is the dimension of the spatial domain. Some numerical examples are presented.

## [04537] Implementation and Application of Virtual Element Method in FEALPy

**Format :** Talk at Waseda University

**Author(s) :** Huayi Wei HUAYI WEI (Xiangtan University )

**Abstract :** The virtual element method is a novel numerical solution technique for PDEs. It can be considered an extension of the finite element method to polygonal or polyhedral meshes. Due to its novelty, the program implementation of this method differs significantly from that of the traditional finite element method. Unfortunately, there are relatively few open-source program implementations available. FEALPy is an open-source numerical solution algorithm library for PDEs. It is built entirely on Python's basic scientific computing module and provides rich mesh data structures, meshes adaptive algorithms, and partial differential equation numerical discrete algorithms. This report primarily focuses on the design and implementation of the virtual element method in FEALPy, along with several typical application examples.

## [05586] Convergence of an AWG method for indefinite time-harmonic Maxwell equations

**Format :** Talk at Waseda University

**Author(s) :** Yingying Xie (Guangzhou University)Liuqiang Zhong (South China Normal University)Ming Tang (South China Normal University)

**Abstract :** In this talk, an adaptive weak Galerkin (AWG) method for indefinite time-harmonic Maxwell equations is studied. Firstly, a residual type a posteriori error estimator is presented and analyzed. Then, a quasi-orthogonality is presented by introducing interpolator operators. And the convergence of AWG algorithm is also proved. Finally, some numerical experiments is provided to support the theoretical results.

## [04955] High order stable generalized finite element method for interface problems

**Format :** Talk at Waseda University

**Author(s) :** Qinghui Zhang (Harbin Institute of Technology, Shenzhen)

**Abstract :** Generalized or Extended Finite Element Methods (GFEM/XFEM) of degree 1 (linear elements) for interface problems have been reported in the literature; they (i) yield optimal order of convergence in energy norm, i.e.,  $O(h)$ , (ii) are stable in a sense that conditioning is not worse than that of the standard FEM, and (iii) are robust in that the conditioning does not deteriorate as interface curves are close to boundaries of underlying elements. However, higher order GFEM/XFEM with the properties (i)-(iii) have not been successfully addressed yet. Various enrichment schemes for GFEM/XFEM based on D or DP\_k (D is a distance function or the absolute value of level set function, and P\_k is the polynomial basis of degree k) have been reported to obtain higher order convergence, but they are not stable or robust in general; in fact, they even may not yield the optimal orders of convergence. In this talk, we propose a stable GFEM/XFEM of degree 2 (SGFEM2) for the interface problems, where we use the enrichment scheme based on  $D\{1, x, y\}$ , instead of  $D$  or  $D\{x, y, x^2, xy, y^2\}$  in the literature. We prove that the SGFEM2 yields the optimal order of convergence, i.e.,  $O(h^2)$ , for the interface problems with curved (smooth) interfaces. A local principal component analysis technique is proposed, which ensures that the SGFEM2 is stable and robust. Numerical experiments for straight and curved interfaces have been presented to illuminate these properties.

## [01718] On SDP relaxations of polynomial optimization

**Session Time & Room :**

01718 (1/2) : 3D (Aug.23, 15:30-17:10) @D501

01718 (2/2) : 3E (Aug.23, 17:40-19:20) @D501

**Type :** Proposal of Minisymposium

**Abstract :** TBA

**Organizer(s) :** Sunyoung Kim, Kim-Chuan Toh

**Classification :** 90-08, convex programming, semidefinite programming

**Minisymposium Program :**


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01718 (1/2) : 3D @D501 [Chair: Kim-Chuan Toh]

### **[01976] Tightness conditions of SDP relaxation for QCQPs with bipartite graph structure**

**Format :** Talk at Waseda University

**Author(s) :** Godai Azuma (Tokyo Institute of Technology)Mituhiro Fukuda (Federal University of ABC)Sunyoung Kim (Ewha Womans University)Makoto Yamashita (Tokyo Institute of Technology)

**Abstract :** We discuss a tightness condition of SDP, semidefinite programming, relaxation for QCQPs, quadratically-constrained quadratic programming problems, with bipartite graph structure, and this result generalizes that a condition that the SDP relaxation is tight for QCQPs with diagonal matrices due to Burer and Ye, and a condition based the signs of the elements in input data matrices analyzed by Sojoudi and Lavaei. Our condition to check the tightness of SDP relaxation demands to solve SDP systems, but it requires weaker assumptions than Sojoudi and Lavaei. Our approach also gives another proof for the tightness of SDP relaxations for QCQPs with off-diagonal nonpositive elements by converting such QCQPs into QCQPs with bipartite graph structure.

### **[02464] Equivalent Sufficient Conditions for Exact SDP Relaxation and the Saddle Point of Lagrangian Function of QCQP**

**Format :** Talk at Waseda University

**Author(s) :** Sunyoung Kim (Ewha W. University)Masakazu Kojima (Chuo University)

**Abstract :** We study global optimality conditions for general quadratically constrained quadratic program (QCQP). For NP-hard nonconvex QCQP, there has been a great interest in the class of QCQPs whose global optimality can be obtained via convex relaxations. The exactness of optimal solutions of QCQP can determined by several methods: First, the optimal solution  $X \in S_+^n$  of the semidefinite (SDP) relaxation of nonconvex QCQP is exact if its rank is 1 or the rank of dual optimal solution of the SDP relaxation is n-1 under strong duality. Second, the global optimality of solutions of QCQP can be also determined by the saddle point of the Lagrangian function of QCQP. Third, second-order sufficient condition for the global optimality can also be used. We examine the relationship among the three conditions and prove their equivalence. A QCQP instance is provided to illustrate the equivalent conditions.

### **[02214] Approximation Hierarchies for Copositive Cone over Symmetric Cone**

**Format :** Talk at Waseda University

**Author(s) :** Mitsuhiro Nishijima (Tokyo Institute of Technology)Kazuhide Nakata (Tokyo Institute of Technology)

**Abstract :** We first provide an inner-approximation hierarchy described by a sum-of-squares constraint for the copositive cone over a general symmetric cone. We second provide inner- and outer-approximation hierarchies described by semidefinite but not by sum-of-squares constraints for the copositive cone over the direct product of a nonnegative orthant and a second-order cone. We also compare them with existing hierarchies. Numerical experiments show that, by combining them, we can solve copositive programming problems more accurately and efficiently.

### **[02008] An inexact projected gradient method with rounding and lifting for rank-one semidefinite relaxation of polynomial optimization**

**Format :** Talk at Waseda University

**Author(s) :** Kim-Chuan Toh (National University of Singapore)Heng Yang (Harvard University)Ling Liang (National University of Singapore)Luca Carlone (MIT)

**Abstract :**

We consider solving high-order semidefinite programming (SDP) relaxations of polynomial optimization problems (POPs) that often admit degenerate rank-one optimal solutions. We propose a new algorithmic framework that uses an inexact projected gradient method for solving the SDP, together with acceleration by taking long, but safeguarded, rank-one steps generated by fast local solver for the underlying POP. Our framework

achieves state-of-the-art efficiency, scalability, and robustness in solving degenerate rank-one SDPs to high accuracy, even with millions of equality constraints.

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01718 (2/2) : 3E @D501

## [01768] Computer-assisted proofs in differential equations

**Session Time & Room :**

01768 (1/4) : 3C (Aug.23, 13:20-15:00) @G405

01768 (2/4) : 3D (Aug.23, 15:30-17:10) @G405

01768 (3/4) : 3E (Aug.23, 17:40-19:20) @G405

01768 (4/4) : 4C (Aug.24, 13:20-15:00) @G405

**Type :** Proposal of Minisymposium

**Abstract :** Several phenomena from biology, physics and chemistry are described by differential equations. While the presence of nonlinearities complicates the mathematical analysis, the challenges are greater for PDEs and delay equations, which are infinite dimensional. Numerics have therefore become the primary tool used by scientists, which leads to the question of validity of the outputs. To address this, the field of computer-assisted proofs (CAPs) in dynamics emerged at the intersection of scientific computing, nonlinear, numerical and functional analysis and approximation theory. This minisymposium will bring experts describing novel CAPs techniques to study cutting-edge problems in finite and infinite dimensional differential equations.

**Organizer(s) :** Jean-Philippe Lessard, Akitoshi Takayasu, Nobito Yamamoto

**Classification :** 35-XX, 37-XX, 65-XX, 34-XX, 65Gxx

**Minisymposium Program :**

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01768 (1/4) : 3C @G405 [Chair: Akitoshi Takayasu]

## [04529] Numerical verification methods for ODEs with conservative quantity

**Format :** Talk at Waseda University

**Author(s) :** Nobito Yamamoto (The University of Electro-Communications)Koki Nitta (The University of Electro-Communications)

**Abstract :** We are treating ODEs with conservative quantity and interested in proving existence of time-global solutions remaining in a given sphere with common points on the surface. There is difficulty in computing the solution orbits for a long time due to drift between solutions of conservative systems.

Our method is based on verified computation of the conservative quantity and the flow on the surface of the sphere. Numerical examples derived from Schroedinger equation will be shown.

## [04834] Computer-assisted Existence Proofs for Navier-Stokes Equations on an Unbounded Strip with Obstacle

**Format :** Talk at Waseda University

**Author(s) :** Michael Plum (Karlsruhe Institute of Technology)Jonathan Wunderlich (Karlsruhe Institute of Technology)

**Abstract :** The incompressible stationary 2D Navier-Stokes equations are considered on an unbounded strip domain with a compact obstacle. A computer-assisted existence and enclosure result for the velocity (in a suitable divergence-free Sobolev space) is presented.

Starting from a numerical approximate solution (computed with divergence-free finite elements), we determine a bound for its defect and a norm bound for the inverse of the linearization at the approximate solution. For the latter, bounds for the essential spectrum and for eigenvalues close to zero of an associated self-adjoint operator play a crucial role.

To obtain the desired lower bounds for the eigenvalues below the essential spectrum we use a combination of the Rayleigh-Ritz method, a corollary of the Temple-Lehmann-Goerisch theorem and a homotopy method.

## [04194] Relative equilibria for the n-body problem

**Format :** Talk at Waseda University

**Author(s) :** Warwick Tucker (Monash University)Jordi-Lluis Figueras (Uppsala University)Piotr Zgliczynski (Jagiellonian University)

**Abstract :** We will discuss the classical problem from celestial mechanics of determining the number of relative equilibria a set of planets can display. Several already established results will be presented, as well as a new contribution (in terms of a new proof) for the restricted 4-body problem. We will discuss its possible extensions to harder instances of the general problem.

## [05267] Chaos in Mackey-Glass: computation of transverse homoclinic orbits

**Format :** Talk at Waseda University

**Author(s) :** Olivier Hénot (McGill University)

**Abstract :** The Mackey-Glass equation is a scalar delay differential equation, famous for its rich dynamics. Since 1977, the equation has become a primary example of chaos in infinite dimensions. Yet, a proof of existence of chaotic dynamics remains an open problem.

In this talk, we present a computational method for studying transverse homoclinic orbits for periodic solutions of delay differential equations. The connection is formulated as the zero of a nonlinear map representing a boundary value problem, with boundary conditions in the (finite dimensional) unstable and (infinite dimensional) stable manifolds of the periodic orbit; the transversality of the intersection is a by-product of the invertibility of the Fréchet derivative of the map. This technique is designed to be amenable for computer-assisted proofs through a Newton-Kantorovich type argument. As a notable illustration, we compute a transverse homoclinic orbit in the Mackey-Glass equation.

01768 (2/4) : 3D @G405 [Chair: Jean-Philippe Lessard]

## [05182] Smooth imploding solutions for 3D compressible fluids

**Format :** Talk at Waseda University

**Author(s) :** Javier Gomez Serrano (Brown University)

**Abstract :** In this talk I will present results on singularity formation for the 3D isentropic compressible Euler and Navier-Stokes equations for ideal gases. These equations describe the motion of a compressible ideal gas, which is characterized by a parameter called the adiabatic constant. Finite time singularities for generic adiabatic constants were found in the recent breakthrough of Merle, Raphaël, Rodnianski and Szeftel. Our results allow us to drop the genericity assumption and construct smooth self-similar profiles for all values of the adiabatic constant. In particular, we will construct the first smooth self-similar profile for a monoatomic gas. Part of the proof is very delicate and requires a computer-assisted analysis. Joint work with Tristan Buckmaster and Gonzalo Cao-Labora.

## [02910] Computer-assisted proofs of localized patterns in the planar Swift-Hohenberg equation

**Format :** Talk at Waseda University

**Author(s) :** Matthieu Cadiot (McGill University)Jean-Philippe Lessard (McGill University)Jean-Christophe Nave (McGill University)

**Abstract :** In this talk, I will present computer-assisted proofs of stationary localized patterns in the planar Swift-Hohenberg equation. Using a Newton-Kantorovich approach, we develop a numerical method to prove local existence and uniqueness of strong solutions in  $\mathbb{R}^m$ . In particular, I will explain how we manage to approximate the inverse of the linearization of the PDE around some approximated solution. Finally, I will expose the numerical details of some specific computer-assisted proofs.

## [05035] Rigorous computation of Poincare maps

**Format :** Talk at Waseda University

**Author(s) :** Daniel Wilczak (Jagiellonian University)Tomasz Kapela (Jagiellonian University)Piotr Zgliczyński (Jagiellonian University)

**Abstract :** We present recent advances on interval methods for rigorous computation of Poincare maps. We also discuss the impact of choice of Poincare section and coordinate system on obtained bounds for computing Poincare map nearby fixed points.

## [02908] Validation of Elliptic Invariant Tori in Hamiltonian Systems

**Format :** Talk at Waseda University

**Author(s) :** Chiara Caracciolo (Uppsala University)

**Abstract :** The applicability of KAM theorem to realistic physical problems can be significantly improved by CAPs. These proofs exploit the explicit computation of approximately invariant solutions by the mean of normal forms or parametrization methods. I will discuss the extension of these techniques to lower-dimensional elliptic tori and present an algorithm based on a parametrization method. I will discuss the main benefits of this technique and how it can be made completely rigorous.

Based on joint works with J-Ll. Figueras, A. Haro, U. Locatelli.

01768 (3/4) : 3E @G405 [Chair: Nobito Yamamoto]

## [03720] Validated Numerics for divergent series via the Borel Transform

**Format :** Talk at Waseda University

**Author(s) :** Jason Desmond Mireles James (Florida Atlantic University)

**Abstract :** Parabolic invariant manifolds are associated with fixed points of diffeomorphisms which have one as an eigenvalue of the linearization, or equilibrium solutions of differential equations which have zero as an eigenvalue. Supposing that the map or vector field is real analytic, It is well known (for example Baldoma and Haro, 2008) that while the Taylor expansion of the manifold may diverge, it typically does so in a Gevrey fashion. That is, the power series coefficients diverge like a factorial. In this case, some truncations of the divergent series may still provide useful approximation, and it is desirable to have quantitative bounds on the errors. This is in fact necessary if the expansion is going to be used as an ingredient of a subsequent computer assisted proof.

I will discuss a method for obtaining such bounds based on Borel resummation. The idea is that the Borel transform of the conjugacy equation describing the parabolic manifold has much nicer properties than the original equation. For example the transformed equation typically has analytic solutions. I will discuss methods for solving the transformed equation using validated numerics. If one can analytically continue this solution (in a process similar to numerical integration) to an open set covering the positive real axis in the complex Borel Plane, then it is possible to take a Laplace transform, recovering the solution to the original problem. This procedure also leads to validated computer assisted error bounds.

## [04398] Characterising blenders via covering relations and cone conditions

**Format :** Talk at Waseda University

**Author(s) :** Hinke M Osinga (University of Auckland)Bernd Krauskopf (University of Auckland)Piotr Zgliczynski (Jagiellonian University)Maciej Capinski (AGH University of Science and Technology)

**Abstract :** A blender is an invariant hyperbolic set of a diffeomorphism with the property that its stable or unstable manifold has a dimension larger than expected from the underlying hyperbolic splitting. We present a characterisation of a blender based on the correct topological alignment of sets in combination with the propagation of cones. It is applicable to multidimensional blenders in ambient phase spaces of any dimension. The required conditions can be verified by checking properties of a single iterate of the diffeomorphism, which is achieved by positioning the required sets in such a way that they form a suitable sequence of coverings. This setup is flexible and allows for a rigorous, interval arithmetic based, computer assisted validation.

## [03900] Validated integration of semilinear parabolic PDEs

**Format :** Talk at Waseda University

**Author(s) :** Maxime Breden (Ecole polytechnique)Jan Bouwe van den Berg (VU Amsterdam)Ray Sheombarsing (VU Amsterdam)

**Abstract :** Integrating evolutionary partial differential equations (PDEs) is an essential ingredient for studying the

dynamics of the solutions. Indeed, simulations are at the core of scientific computing, but their mathematical reliability is often difficult to quantify, especially when one is interested in the output of a given simulation, rather than in the asymptotic regime where the discretization parameter tends to zero. In this paper we present a computer-assisted proof methodology to perform rigorous time integration for scalar semilinear parabolic PDEs with periodic boundary conditions. We formulate an equivalent zero-finding problem based on a variations of constants formula in Fourier space. Using Chebyshev interpolation and domain decomposition, we then finish the proof with a Newton-Kantorovich type argument. The final output of this procedure is a proof of existence of an orbit, together with guaranteed error bounds between this orbit and a numerically computed approximation. We illustrate the versatility of the approach with results for the Fisher equation, the Swift-Hohenberg equation, the Ohta-Kawasaki equation and the Kuramoto-Sivashinsky equation. We expect that this rigorous integrator can form the basis for studying boundary value problems for connecting orbits in partial differential equations.

## [05270] Validated dynamics in neural networks: towards chaos

**Format :** Talk at Waseda University

**Author(s) :** Elena Queirolo (TUM)

**Abstract :** Neural networks, a class of machine learning algorithms, can be interpreted as dynamical systems and can be studied by dynamical techniques. Here, we use validation techniques to understand how the reliability of the algorithm relates to dynamical behaviours. In particular, we want to investigate the connection between chaos and reliability. First, we prove or disprove the existence of chaos in a given neural net, then we draw behavioural conclusions based on its existence.

01768 (4/4) : 4C @G405 [Chair: Akitoshi Takayasu]

## [05292] Global Dynamics and Blowup in Some Quadratic PDEs

**Format :** Talk at Waseda University

**Author(s) :** Jonathan Jaquette Jean-Philippe Lessard (McGill University)Akitoshi Takayasu (University of Tsukuba)

**Abstract :** Conservation laws and Lyapunov functions are powerful tools for proving the global existence of stability of solutions, but for many complex systems these tools are insufficient to completely understand non-perturbative dynamics. In this talk I will discuss a complex-scalar PDE which may be seen as a toy model for vortex stretching in fluid flow, and cannot be neatly categorized as conservative nor dissipative.

In a recent series of papers we have shown that this equation exhibits rich dynamical behavior that exist globally in time: non-trivial equilibria, homoclinic orbits, heteroclinic orbits, and integrable subsystems foliated by periodic orbits. On the other side of the coin, we show several mechanisms by which solutions can blowup. I will discuss these results, and current work toward understanding unstable blowup.

## [05275] Worrisome Properties of Symbolic Representations of Deep Neural Network Controllers

**Format :** Talk at Waseda University

**Author(s) :** Jacek Cyranka (Warsaw University)Kevin Church ( Université de Montréal )Jean-Philippe Lessard (McGill University)

**Abstract :** We studied dynamics of simple controlled problems like Pendulum and CartPole, where the controllers were trained using reinforcement learning algorithms. We raise concerns about symbolic controllers' robustness.

A typical symbolic controller reaching high mean return values still generates an abundance of unstabilized solutions, which is highly undesirable property, easily exploitable by an adversary. We provide an algorithm for a systematic robustness study and prove the unstabilized solutions and periodic orbits, using a computer-assisted proof methodology.

## [05090] A rigorous integrator and global existence for higher-dimensional semilinear parabolic PDEs via semigroup theory

**Format :** Talk at Waseda University

**Author(s) :** Gabriel William Duchesne (McGill)

**Abstract :**

In this talk, we introduce a general constructive method to compute solutions of initial and boundary value problems of semilinear parabolic partial differential equations via semigroup theory and computer-assisted proofs.

We will present techniques to prove the global existence of solutions in the 2D/3D Swift-Hohenberg equation and to prove the existence of a solution of a projected boundary value problem in the 2D Ohta-Kawasaki equation.

## [01800] Numerical methods for fluid-structure interaction and poroelasticity

### **Session Time & Room :**

01800 (1/2) : 2D (Aug.22, 15:30-17:10) @E820

01800 (2/2) : 2E (Aug.22, 17:40-19:20) @E820

### **Type :** Proposal of Minisymposium

**Abstract :** Fluid-structure interaction problems arise in many applications. In biomedicine, such models are used to describe the interaction between blood and arterial walls. Such models have also been used to describe the interaction between blood flow and biodegradable stents, blood flow in patient-specific models of abdominal aortas containing aneurysms, and blood flow and oxygen transport in a bioartificial pancreas. Other applications include geomechanics and aerodynamics. When a deformable structure is porous and allows flow through it, poroelastic models are commonly used to describe its behavior. The numerical simulation of fluid-elastic/poroelastic structure interaction problems has received considerable attention, but still remains a significant challenge in the mathematical and computational sciences. Main difficulties stem from the intricate multiphysics nature of the problem, and strong nonlinearities. This minisymposium focuses on numerical methods for fluid-elastic or poroelastic structure interaction problems and applications. Possible topics include but are not limited to: 1) partitioned and monolithic numerical methods, 2) porous and poroelastic medium flow, 3) mathematical and numerical analysis, and 4) validation and verification of numerical solvers.

**Organizer(s) :** Martina Bukac, Suncica Canic

**Classification :** 74F10, 76S05, 65M60, 76Z05

### **Minisymposium Program :**

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01800 (1/2) : 2D @E820 [Chair: Martina Bučač]

## [03958] Space-time domain decomposition approach for Stoke flow coupled with poroelasticity

**Format :** Talk at Waseda University

**Author(s) :** Hyesuk Lee (Clemson University) Hemanta Kunwar (Clemson University)

**Abstract :** We consider decoupling iterative algorithms based on domain decomposition for the time-dependent Stokes-Biot model, in which different time steps can be used in the flow region and the poroelastic medium. The coupled system is formulated as a space-time interface problem based on interface conditions. The interface problem is then solved by an iterative method which involves the parallel solution of time-dependent homogeneous Stokes and Biot problems. Consequently, local discretization in both space and time can be used to handle multiphysics systems efficiently. Numerical results with nonconforming time grids are presented to illustrate the performance of the proposed methods.

## [04129] Two-field any-order finite element solvers for poroelasticity problems

**Format :** Talk at Waseda University

**Author(s) :** Jiangguo James Liu (Colorado State University )

**Abstract :** In this talk, we present a family of 2-field finite element solvers for poroelasticity problems based on weak Galerkin (WG) spatial discretizations and the backward differentiation formulas (BDF) temporal discretization. In particular, both primal variables (fluid pressure and solid displacement) are approximated by WG degree  $k \geq 0$  (scalar or vector) polynomial shape functions defined separately in element interiors and on edges of a quadrilateral mesh. The discrete weak gradients of WG basis functions are constructed in certain broken Arbogast-Correa spaces (of vectors or matrices). The discrete weak gradients, strains, and divergences will be utilized to approximate their continuous counterparts in the variational formulations. Degree- $k$  WG polynomials

and BDF(k+1) are combined to develop time-marching schemes for linear poroelasticity. This combination results in a good balance of spatial and temporal discretizations. Numerical experiments on benchmarks will be presented to demonstrate the efficiency and flexibility of these new solvers. Extension to nonlinear poroelasticity problems will be discussed also. This is a joint work with Simon Tavener (Colorado State University, USA), Ruishu Wang (Jilin University, China), and Zhuoran Wang (Sun Yat-sen University, China).

## [04672] A mathematical framework for poro-viso-elastic models

**Format :** Talk at Waseda University

**Author(s) :** Justin Thomas Webster (University of Maryland, Baltimore County)

**Abstract :** Recent works in poroelasticity have included viscous structural effects. Here, we clarify mathematical properties of linear, quasi-static Biot systems with the addition of Kelvin-Voigt viscoelasticity. We demonstrate time-regularization and dissipative effects of viscoelasticity through a priori estimates. We use the full system, as well as the framework of implicit, degenerate evolutions. Precise statements of admissible initial conditions in each scenario are given.

## [04316] An energy stable second-order method for three-phase flows

**Format :** Talk at Waseda University

**Author(s) :** Catalin Trenchea (University of Pittsburgh)Giselle Sosa Jones (Oakland University)

**Abstract :** We present a time-stepping scheme for the numerical approximation of a thermodynamically consistent model of incompressible and immiscible three-phase flow in porous media, with an intrinsic free energy dissipation law.

The model consists of three nonlinear degenerate parabolic equations for the saturations of each phase.

We prove that the proposed scheme is second-order accurate, and preserves the discrete free energy dissipation.

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01800 (2/2) : 2E @E820 [Chair: Martina Bukač]

## [04829] Cell-Based Numerical Approach to Evaluate CTC Binding Behavior in Microfluidic Device

**Format :** Talk at Waseda University

**Author(s) :** YIFAN Wang (Texas Tech University)

**Abstract :** Circulating tumor cells (CTCs) are malignant cells that break free from the primary tumor and enter the bloodstream. Early detection of CTCs is crucial for diagnosis, but challenging because they are infrequent in blood samples. Microfluidic devices offer a promising detection technique, either actively enriching CTCs through external fields or passively separating them from other cells based on physical properties. A microfluidic device has been proposed by our collaborator at Texas Tech University to isolate CTCs from blood samples, with different micro-post sizes and layouts tested to optimize capture efficiency. However, the complex transport and adhesion behaviors of CTCs in blood cell suspensions remain incompletely understood. Here, we present a cell-based numerical approach based on the Lattice Boltzmann method to evaluate the binding behavior and trajectories of CTCs under different flow conditions, including cell size and coating density, microfluidic design, and cell collisions. Our validated results are used to improve the device design.

## [02971] A Banach spaces-based fully-mixed formulation for the Navier-Stokes/Darcy coupled problem

**Format :** Talk at Waseda University

**Author(s) :** Segundo Villa Fuentes (Monash University)Ricardo Oyarzúa (Universidad del Bío-Bío)Sergio Caucao (Universidad Católica de la Santísima Concepción)

**Abstract :** In this work we present and analyze a fully-mixed formulation for the coupling Navier-Stokes/Darcy equations.

Our approach is based on the introduction of a modified pseudostress tensor in the Navier-Stokes equations for the fluid, whereas the standard dual-mixed formulation for the Darcy model is considered. With this, we obtain a Banach spaces-based mixed variational formulation and a twofold saddle point structure.

Fixed-point strategy, together with the Banach–Nečas–Babuška and Banach's fixed point theorems, are employed to prove the well-posedness of the continuous and discrete formulations.

## [03829] Numerical simulation of the time-fractional Navier-Stokes-Fokker-Planck (tfNSFP) equation

**Format :** Talk at Waseda University

**Author(s) :** Jonas Beddrich (Technical University of Munich)Endre Süli (University of Oxford)Barbara Wohlmuth (Technical University of Munich)

**Abstract :** The tfNSFP system describes the flow of dilute polymeric fluids. It is attractive as it enhances standard models for the viscoelasticity of polymer molecules by accounting for memory effects. The problem is challenging since it is non-local in time and defined on the Cartesian product of two d-dimensional spaces. We present a numerical method that combines a rational approximation approach, a space-splitting approach, and the Hermite spectral method to solve the tfNSFP equation.

## [01834] Structure analysis and dynamics modelling in graphs and networks

**Session Time & Room :**

01834 (1/2) : 3C (Aug.23, 13:20-15:00) @G304

01834 (2/2) : 3D (Aug.23, 15:30-17:10) @G304

**Type :** Proposal of Minisymposium

**Abstract :** In recent years, research on graphs and networks has received much attention, and it has emerged in the application of channel coding, biomedicine, social governance, and other fields. The mini-symposium will focus on structural analysis and dynamics modelling in complex networks, including influence maximization of high-order networks, evolutionary games, etc.

**Organizer(s) :** Cunquan Qu, Chenlu Ji, Fang Wang

**Classification :** 05Cxx, 91Dxx, 91Gxx, Network Science; Evolutionary Game Theory

**Minisymposium Program :**

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01834 (1/2) : 3C @G304 [Chair: Cunquan QU]

## [03989] Evolutionary Game Theory on Dynamic Networks

**Format :** Online Talk on Zoom

**Author(s) :** Qi Su (University of St Andrews)Alex McAvoy (University of Pennsylvania)Joshua B. Plotkin (University of Pennsylvania)

**Abstract :** The study of the evolution of cooperative behavior on static networks helps to understand how population structure can facilitate the spread of prosocial traits. However, real-world interactions are usually transient and subject to external restructuring, making the study of strategic behavior on dynamic networks difficult. This study provides an analytical treatment of cooperation on dynamic networks and demonstrates that transitions among network structures can promote the spread of cooperation, even if individual social networks inhibit it when static. The findings highlight the significant impact of dynamic social structures on the evolution of prosocial traits.

## [02059] An efficient adaptive degree-based heuristic algorithm for influence maximization in hypergraphs

**Format :** Online Talk on Zoom

**Author(s) :** Xiu-Xiu Zhan (Hangzhou Normal University)

**Abstract :** Influence maximization (IM) has shown wide applicability in immense fields over the past decades. Previous researches on IM mainly focused on the dyadic relationship but lacked the consideration of higher-order relationship between entities, which has been constantly revealed in many real systems. An adaptive degree-based heuristic algorithm, i.e., Hyper Adaptive Degree Pruning (HADP) which aims to iteratively select nodes with low influence overlap as seeds, is proposed in this work to tackle the IM problem in hypergraphs. Furthermore, we extend algorithms from ordinary networks as baselines. Results on 8 empirical hypergraphs show that HADP surpasses the baselines in terms of both effectiveness and efficiency with a maximally 46.02% improvement. Moreover, we test the effectiveness of our algorithm on synthetic hypergraphs generated by different degree

heterogeneity. It shows that the improvement of our algorithm effectiveness increases from 2.66% to 14.67% with the increase of degree heterogeneity, which indicates that HADP shows high performance especially in hypergraphs with high heterogeneity, which is ubiquitous in real-world systems.

## [04046] Identifying vital nodes through augmented random walks on higher-order networks

**Format :** Online Talk on Zoom

**Author(s) :** Xiao-Long Ren (Yangtze Delta Region Institute (Huzhou), University of Electronic Science and Technology of China)

**Abstract :** Identifying vital nodes is still unclear in the study of higher-order networks. We introduce a multi-order graph obtained by incorporating the higher-order bipartite graph and the classical pairwise and propose a Higher-order Augmented Random Walk model. Our model provides a new approach for ranking nodes at multiple scales. Our method outperforms other indicators in identifying vital nodes and can scale to various tasks in complex networks, including the information spread maximization and network dismantling problem.

## [04449] Emergence of Cooperation Through Coevolving Time Scale in Spatial Prisoner's Dilemma

**Format :** Online Talk on Zoom

**Author(s) :** Zhihai Rong (Donghua University)

**Abstract :** Understanding the emergence of cooperation is a challenging problem and has drawn a wide attention from various fields including sociology, economics and biology. Evolutional game theory provides a powerful framework for investigating this problem. In the traditional networked evolutionary game theory, most researchers usually assume an individual will immediately update its strategy after one round of game with its neighbors. However, in the social and biological systems the strategy-selection time scale may be slower than the interaction time scale, i.e., an individual will hold its current strategy and play several rounds of game with its neighbors, and then update its behavior. In this talk, I will introduce some results about coevolving time scale in spatial Prisoner's dilemma. When the individuals can adjust their strategy-selection time scale according to some rules, optimal cooperation can be induced by proper adaptive rate in the strategy-selection time scale. The results are analyzed through the spatial pattern and feedback mechanism of individual behavior. This investigation may have potential implications in the design of consensus protocol in multi-agent systems.

01834 (2/2) : 3D @G304 [Chair: Chenlu JI]

## [01988] information-opinion dynamics on social multilayer networks

**Format :** Online Talk on Zoom

**Author(s) :** Fei Jing (City University of Hong Kong)

**Abstract :** Here we model these two phenomena as a co-evolution dynamics of information and public opinion on heterogeneous multiplex networks, including a few extreme individuals with constant opinions and a vast majority of general individuals with vacillating views.

## [04619] Characterizing Cycle Structure in Complex Networks

**Format :** Online Talk on Zoom

**Author(s) :** Tianlong Fan (University of Fribourg)

**Abstract :** A cycle is the simplest structure that brings redundant paths in network connectivity and feedback effects in network dynamics. In this work, we define the cycle number matrix, and the cycle ratio, an index that quantifies node importance. Numerical experiments on identifying vital nodes for network connectivity and synchronization and maximizing the early reach of spreading show that the cycle ratio performs overall better than other benchmarks.

## [03130] Collaborative deep learning framework for network inference and dynamical prediction

**Format :** Online Talk on Zoom

**Author(s) :** Xiao Ding (Anhui University)

**Abstract :** How to use incomplete data to infer network structure as well as predict the dynamics simultaneously is a meaningful and challenging question. To this end, we develop a COllaborative deep learning framework for Network inference and Dynamical prediction (CoND). Extensive experiments demonstrate that CoND outperforms the baseline methods regarding both tasks for different networks and dynamical models. To further validate the effectiveness of CoND, we demonstrate the superior performance of CoND on two real datasets.

## [05541] Multichannel game on structured populations

**Format :** Online Talk on Zoom

**Author(s) :** Fanpeng Song (Shandong University)

**Abstract :** In this talk, we introduce a framework of multichannel game on structured populations and explore the effect of topological properties to the evolutionary dynamics. Significantly, we find that the heterogeneity of populations is detrimental to the dynamics, especially in BA networks. In addition, modest population size and high interaction are in favor of the dynamics. These results are meaningful for the research on cooperation and human development.

# [01858] Interplay among Manifold Learning, Stochastic Calculus, and Volatility Estimation

**Session Time & Room :**

01858 (1/3) : 2E (Aug.22, 17:40-19:20) @E503

01858 (2/3) : 3C (Aug.23, 13:20-15:00) @E503

01858 (3/3) : 3D (Aug.23, 15:30-17:10) @E503

**Type :** Proposal of Minisymposium

**Abstract :** We will review recent advances in Manifold Learning inviting top researchers in this field, and also invite some speakers who will deliver recent developments in Mallivin-Mancino's Fourier estimation method for estimating the "spot volatility process", and its application to the estimation of the diffusion matrix. The aim of the mini-symposium is to forecast how we can proceed to combine these two methods to refine the existing results and reach a new stage.

**Organizer(s) :** Jiro Akahori, Hau-Tieng Wu

**Classification :** 62G05, 60F99, 60H30, 53A99, 91G70

**Minisymposium Program :**

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01858 (1/3) : 2E @E503 [Chair: Hau-Tieng Wu]

## [02841] Convergence of Hessian estimator from random samples on a manifold

**Format :** Talk at Waseda University

**Author(s) :** Chih-Wei Chen (National Sun Yat-sen University)Hau-Tieng Wu (Duke University)

**Abstract :** We provide a systematic convergence analysis of the Hessian operator estimator from random samples supported on a low dimensional manifold. We show that the impact of the nonuniform sampling and the curvature on the widely applied Hessian operator estimator is asymptotically negligible.

## [02848] Limit Theorems for the Positive Semidefinite Modification of Malliavin-Mancino Estimator for the Spot Volatility Process

**Format :** Talk at Waseda University

**Author(s) :** Reika Kambara (Nomura Asset Management Co., Ltd.)

**Abstract :** In this talk, the consistency, and the asymptotic normality of the class of Fourier-type estimators introduced by Akahori et al. will be discussed. The class, parameterized by a sequence of probability measures, is a modification of the Fourier series method introduced by Malliavin and Mancino, modified so that the estimator is positive semidefinite.

## [04489] Convergence of Laplacian and its rate for submanifolds that are not necessarily smooth

**Format :** Talk at Waseda University

**Author(s) :** Masayuki Aino (Proxima Technology)

**Abstract :** The continuous limit of Laplacian Eigenmaps gives the eigenfunctions of the Laplacian on submanifolds in Euclidean space .

Such studies have been based on the assumption that a quantity called Reach is bounded from below.

Submanifolds with non-differentiable points cannot be approximated under such an assumption.

In this talk, I discuss the convergence of Laplacian Eigenmaps and its rates when the Reach assumption is replaced by a weaker assumption such that non-differentiable points can appear.

01858 (2/3) : 3C @E503 [Chair: Hiroshi Kawabi]

## [02761] On excursions inside an excursion

**Format :** Talk at Waseda University

**Author(s) :** Ju-Yi Yen (University of Cincinnati)

**Abstract :** The distribution of ranked heights of excursions of a Brownian bridge is given by Pitman and Yor in [1].

In this work, we consider excursions of a Brownian

excursion above a random level  $x$ , where  $x$  is the value of the excursion at an independent uniform time on \$

## [0,1]\$. We analyze the maximum heights of these

excursions as Pitman and Yor did for excursions of a Brownian bridge.

[1] J. Pitman and M. Yor. On the distribution of ranked heights of excursions of a Brownian bridge. Ann. Probab., 29(1):361–384, 2001.

## [02842] Diffusion Estimation with Fourier-Malliavin Method

**Format :** Talk at Waseda University

**Author(s) :** Takatoshi Hirano Jiro Akahori (Ritsumeikan university)Simona Sanfelici (Parma university)

**Abstract :** In this talk, the estimation of the diffusion coefficient of the solution to a stochastic differential equation using Fourier estimation method proposed by P. Malliavin and M.E. Mancino is discussed.

## [02849] Statistical Analysis with Geodesics and Curvature in Data Space

**Format :** Talk at Waseda University

**Author(s) :** Kei Kobayashi (Keio University)Henry P. Wynn (London School of Economics)

**Abstract :** We proposed a method to perform data analysis after two types of metric transformation of the data space. The first transformation is based on the powered density integration and can be implemented approximately using an empirical graph. The second transformation corresponds to computing the extrinsic distance after embedding the data space into a metric cone. We proved both transformations monotonically change the curvature of the data space, but in different ways.

01858 (3/3) : 3D @E503 [Chair: Jiro Akahori]

## [02840] A Quantitative Central Limit Theorem arising from Time-Frequency Analysis

**Format :** Talk at Waseda University

**Author(s) :** Gi-Ren Liu (National Cheng Kung University)

**Abstract :** In this talk, we will discuss the distribution distance between the output  $F$  of the scattering transform (ST) of a Gaussian process and its scaling limit  $G$ .

ST is a nonlinear transformation that involves a sequential interlacing convolution and nonlinear operators, which is motivated to model the convolutional neural network. We will show that the total variation distance between the distributions of the output of ST and a chi-square random variable with one degree of freedom converges to zero at an exponential rate.

For achieving this goal, we derive a recursive formula to represent the nonlinearity of ST by a linear combination of Wiener chaos and then apply the Malliavin calculus and Stein's method to estimate the maximal difference between the expectation values of  $h(F)$  and  $h(G)$  over a specific set of test functions  $h$ .

This talk is based on joint work with Yuan-Chung Sheu (National Yang Ming Chiao Tung University, Taiwan) and Hau-Tieng Wu (Duke University, USA).

## [02846] Market Price-Volatility Simulator

**Format :** Talk at Waseda University

**Author(s) :** Riki Kitano (Ritsumeikan University)

**Abstract :** In this talk, a combination of the Fourier-Malliavin-Mancino method and the Lyons's signature method under a stochastic volatility diffusion setting will be discussed.

## [02733] A graph discretized approximation of diffusions on Riemannian manifolds

**Format :** Talk at Waseda University

**Author(s) :** Hiroshi Kawabi (Keio University)Satoshi Ishiwata (Yamagata University)

**Abstract :** In this talk, we discuss a graph discretized approximation for diffusions on a complete Riemannian manifold  $M$ . More precisely, for a given drifted Schrödinger operator  $\mathcal{A} = -\Delta - b + V$  on  $M$ , we introduce a family of random walks in the flow generated by the drift  $b$  with killing on a sequence of proximity graphs. The drifted Schrödinger semigroup  $\{e^{t\mathcal{A}}\}_{t \geq 0}$  is approximated by discrete semigroups generated by the family of random walks.

# [01868] An introduction of “Journal of Machine Learning” for applied mathematicians

**Session Time & Room :**

01868 (1/2) : 4D (Aug.24, 15:30-17:10) @E818

01868 (2/2) : 4E (Aug.24, 17:40-19:20) @E818

**Type :** Proposal of Minisymposium

**Abstract :** Machine learning is an area characterized by rapid growth, broader impact and diverse audience. It is changing applied mathematics in a fundamentally way. At the same time, there is still a lack of proper venues for publishing research work in machine learning with an applied math orientation. Journal of Machine Learning (JML) is a newly launched journal to provide such a venue. It strives to accommodate both the special features of machine learning mentioned above, as well as the long-held tradition of applied mathematics. In this minisymposium, we invite authors who have published papers in JML to present their work.

**Organizer(s) :** Weinan E, Bin Dong, Arnulf Jentzen, Zhiqin Xu

**Classification :** 68TXX, 68WXX, 65NXX, 65ZXX**Minisymposium Program :**

01868 (1/2) : 4D @E818 [Chair: Zhi-Qin John Xu]

## [02598] Embedding Principle: A Hierarchical Structure of Loss Landscape of Deep Neural Networks

**Format :** Talk at Waseda University**Author(s) :** Yaoyu Zhang (Shanghai Jiao Tong University)

**Abstract :** This talk is about the Embedding Principle of loss landscape of deep neural networks ((NNs)), i.e., loss landscape of an NN "contains" all critical points of all the narrower NNs. We will introduce a general class of embedding operators which map any critical point of a narrower NN to a critical point of the target NN preserving the output. Our results uncover a hierarchical structure of loss landscape special to the deep learning models.

## [02247] Perturbational Complexity and Reinforcement Learning in Reproducing Kernel Hilbert Space

**Format :** Talk at Waseda University**Author(s) :** Jihao Long (Princeton University)

**Abstract :** This talk will offer some fresh insight into the challenge for analyzing reinforcement learning (RL) in a general reproducing kernel Hilbert space (RKHS). We define a quantity called “perturbational complexity by distribution mismatch” and show that the perturbational complexity gives both the lower bound and upper bound of the error for the RL problem in RKHS. We will provide some concrete examples and discuss whether the complexity decays fast or not in these examples.

## [02258] The Random Feature Method for Solving Partial Differential Equations

**Format :** Talk at Waseda University**Author(s) :** Jingrun Chen (University of Science and Technology of China)

**Abstract :** In this presentation, we will give a description of the random feature method for solving partial differential equations, including its basic formulation for both static and time-dependent problems and the application for three dimensional problems with complex geometries.

## [02957] DeePN<sup>2</sup>: A deep learning-based non-Newtonian hydrodynamic model

**Format :** Talk at Waseda University**Author(s) :** Huan Lei Lidong Fang (Michigan State University)Pei Ge (Michigan State University)Lei Zhang (Shanghai Jiao Tong University)Weinan E (Peking University)

**Abstract :** A long standing problem in the modeling of non-Newtonian hydrodynamics of polymeric flows is the availability of reliable and interpretable hydrodynamic models that faithfully encode the underlying micro-scale polymer dynamics. We developed a deep learning-based non-Newtonian hydrodynamic model, DeePN<sup>2</sup>, that enables us to systematically pass the micro-scale structural mechanics information to the macro-scale hydrodynamics for polymer suspensions. The model retains a multi-scaled nature with clear physical interpretation, and strictly preserves the frame-indifference constraints.

01868 (2/2) : 4E @E818 [Chair: Yaoyu Zhang]

## [02982] Generalization ability and memorization phenomenon of distribution learning models

**Format :** Talk at Waseda University**Author(s) :** Hongkang Yang (Princeton University, Program in Applied and Computational Mathematics)

**Abstract :** Generative models and density estimators suffer from the memorization phenomenon (i.e. convergence to the finite training samples) as training time goes to infinity. This deterioration is in contradiction to the empirical success of models such as StableDiffusion and GPT-3. We resolve this paradox by proving that

distribution learning models enjoy implicit regularization during training. Specifically, prior to the onset of memorization, their generalization errors at early-stopping escape from the curse of dimensionality.

## [04035] Approximation of Functionals by Neural Network without Curse of Dimensionality

**Format :** Talk at Waseda University

**Author(s) :** Yahong Yang (The Hong Kong University of Science and Technology)Tianyu Jin (The Hong Kong University of Science and Technology)Yang Xiang (Hong Kong University of Science and Technology)

**Abstract :** In this paper, we establish a neural network to approximate functionals, which are maps from infinite dimensional spaces to finite dimensional spaces. The approximation error of the neural network is  $O(1/\sqrt{m})$  where  $m$  is the size of networks, which overcomes the curse of dimensionality. Then, the proposed method is employed in several numerical experiments, such as evaluating the energy functionals and solving Poisson equations by the aforementioned network at one or a few given points.

## [02256] Approximation of Functionals by Neural Network without Curse of Dimensionality

**Format :** Talk at Waseda University

**Author(s) :** Yahong Yang (Hong Kong University of Science and Technology)Yang Xiang (Hong Kong University of Science and Technology)

**Abstract :** In this paper, we establish a neural network to approximate functionals, which are maps from infinite dimensional spaces to finite dimensional spaces. The approximation error of the neural network is  $O(1/\sqrt{m})$  where  $m$  is the size of networks. In other words, the error of the network is no dependence on the dimensionality respecting to the number of the nodes in neural networks. The key idea of the approximation is to define a Barron space of functionals.

## [02998] Ab-Initio Study of Interacting Fermions at Finite Temperature with Neural Canonical Transformation

**Format :** Talk at Waseda University

**Author(s) :** Hao Xie (Institute of Physics, Chinese Academy of Sciences)Linfeng Zhang (DP Technology/AI for Science Institute)Lei Wang (Institute of Physics, Chinese Academy of Sciences)

**Abstract :** We present a variational density matrix approach to the thermal properties of interacting fermions in the continuum. The variational density matrix is parametrized by a permutation equivariant many-body unitary transformation together with a discrete probabilistic model. The unitary transformation is implemented as a quantum counterpart of neural canonical transformation, which incorporates correlation effects via a flow of fermion coordinates. As the first application, we study electrons in a two-dimensional quantum dot with an interaction-induced crossover from Fermi liquid to Wigner molecule. The present approach provides accurate results in the low-temperature regime, where conventional quantum Monte Carlo methods face severe difficulties due to the fermion sign problem. The approach is general and flexible for further extensions, thus holds the promise to deliver new physical results on strongly correlated fermions in the context of ultracold quantum gases, condensed matter, and warm dense matter physics.

## [01897] New Tools for Nonlinear Time Series Analysis

**Session Time & Room :**

01897 (1/2) : 3D (Aug.23, 15:30-17:10) @F309

01897 (2/2) : 3E (Aug.23, 17:40-19:20) @F309

**Type :** Proposal of Minisymposium

**Abstract :** Nonlinear time series analysis is the study of continuous-valued time series under the working hypothesis that they have been produced by a dynamical system of possibly higher dimensions. This assumption enables us to use methods, such as embedding theorems, and tools, such as Lyapunov exponents and attractor dimensions, that allow capturing data structure and information that traditional statistical approaches cannot.

Other recently developed tools include recurrence plots, complex networks, ordinal patterns, visibility graphs, homology groups, transcripts, and more. This Minisymposium is intended to showcase such tools and provide a discussion forum for researchers in the field.

**Organizer(s)** : Jose M. Amigo, Reik V. Donner

**Classification** : 37M10, 37A50, 60G10, Nonlinear time series analysis

**Minisymposium Program :**

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01897 (1/2) : 3D @F309 [Chair: José M. Amigó]

## [05007] Pattern-based approaches to identifying coupling structures among multivariate time series

**Format** : Talk at Waseda University

**Author(s)** : Reik V. Donner (Magdeburg-Stendal University of Applied Sciences)

**Abstract** : Nonlinear analysis methods based on the occurrences of patterns have recently proven valuable tools for time series analysis. In this talk, I will review some recently developed approaches based on co-occurrence statistics between ordinal patterns, graphlets, or extreme events in multivariate time series and their use for correctly distinguishing direct from indirect coupling in otherwise challenging situations, including examples of variables with poor observability characteristics.

## [03507] Transition network approaches for nonlinear time series analysis

**Format** : Talk at Waseda University

**Author(s)** : Yong Zou (East China Normal University)

**Abstract** : Complex networks are powerful tools for nonlinear time series analysis, which are undergoing fast development in the recent decade. Here we propose a novel way to construct multi-scale transition networks from time series, which are based on coarse-graining partitions of phase space. Using time series from both discrete Henon map and continuous Rössler systems, we demonstrate that the multi-scale transition entropy values of the resulting networks show the same power as the Lyapunov exponents, identifying chaotic transitions successfully. The advantage is that our method works successfully when only a small number of 3–5bins is used for the partition generation, while the traditional static node entropy measures work poorly. Further experimental examples in fMRI and ECG analysis show that these entropy measures are able to characterize different rhythmic states of subjects, showing high potential for time series analysis from complex systems.

## [04058] Persistent homology induced by ordinal patterns for multivariate time series

**Format** : Talk at Waseda University

**Author(s)** : Taichi Haruna (Tokyo Woman's Christian University)

**Abstract** : We present a method to construct a filtered simplicial complex from a given multivariate time series using the intersections of ordinal patterns. The filtered complex reflects information about couplings among individual time series. A measure of the complexity of couplings can be defined from its persistent homology groups. The behavior of the complexity measure is investigated in terms of its mathematical properties and applications to examples.

## [04580] Reconstruction of causal graphs with self loops

**Format** : Online Talk on Zoom

**Author(s)** : X. San Liang (Fudan University)

**Abstract** : Causality analysis is an important problem lying at the heart of science. An endeavor during the past years viewing causality as a real physical notion so as to formulate it from first principles, however, seems to have gone unnoticed. This study introduces to the community this line of work. The resulting formula is transparent, and can be implemented as a computationally very efficient algorithm for application. Different from the previous work along this line, here an algorithm is also implemented to quantify the influence of a unit to itself. While this forms a challenge in some causal inferences, here it comes naturally, and hence the identification of self-loops in a causal graph is fulfilled automatically as the causalities along edges are inferred. To demonstrate the power of the approach, presented here are two applications in extreme situations. The first is a network of multivariate processes buried in heavy noises (with the noise-to-signal ratio exceeding 100), and the second a network with nearly synchronized chaotic oscillators. In both graphs, confounding processes exist. While it seems to be a challenge to reconstruct from given series these causal graphs, an easy application of the algorithm immediately reveals the desideratum. Particularly, the confounding processes have been accurately differentiated.

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01897 (2/2) : 3E @F309 [Chair: Reik V. Donner]

## [03926] Power spectrum estimation for extreme events data

**Format :** Talk at Waseda University

**Author(s) :** Norbert Marwan (Potsdam Institute for Climate Impact Research (PIK))Tobias Braun (Potsdam Institute for Climate Impact Research (PIK))

**Abstract :** The estimation of power spectral density (PSD) of time series is an important task in many quantitative scientific disciplines. However, the estimation of PSD from discrete data, such as extreme event series is challenging. We present a novel approach for the estimation of a PSD of discrete data. Combining the edit distance metric with the Wiener-Khinchin theorem provides a simple yet powerful PSD analysis for discrete time series (e.g., extreme events). This method works directly with the event time series without interpolation or transformation to continuous data. We demonstrate the method's potential on some prototypical examples and on event sequences of atmospheric rivers (AR), narrow filaments of extensive water vapor transport in the lower troposphere. Considering the spatial-temporal event series of ARs over Europe, we investigate the presence of a seasonal cycle as well as periodicities in the multi-annual range for specific regions, likely related to the North-Atlantic Oscillation (NAO).

## [04346] Constructing First Return Maps from Ordinal Partitioning of Time Series

**Format :** Talk at Waseda University

**Author(s) :** Zahra Shahriari (The University of Western Australia)

**Abstract :** We present a robust algorithm for constructing first return maps (FRM) of dynamical systems from time series that does not require embedding. Typically, an FRM is constructed utilizing the time series' maxima or zero-crossings. Our method is based on ordinal partitions, and we use consecutive ordinal symbols to construct the FRM. For each ordinal sequence, we generate a unique FRM and rank them using two entropy-based measures to select the "good" ones.

## [04581] Optimization approaches in analyzing marked point process data

**Format :** Talk at Waseda University

**Author(s) :** Noriyoshi Sukegawa (Hosei University)Shohei Suzuki (Tokyo University of Science)Yoshiko Ikebe (Tokyo University of Science)Yoshito Hirata (University of Tsukuba)

**Abstract :** In this talk, we present an integer programming model for computing a median of a set of marked point processes under an edit distance. The marked point process is a time series of discrete events with marks observed in continuous time. The edit distance is a common metric originated by Victor and Purpura in 1997. We show numerical results on its application in earthquake prediction.

## [02926] Generalized entropies in nonlinear time series analysis

**Format :** Talk at Waseda University

**Author(s) :** Jose M. Amigo (Universidad Miguel Hernandez)

**Abstract :** The concept of entropy plays an important role in both random and deterministic processes. In nonlinear time series analysis, entropy is mostly used to characterize the complexity of the data source. To this end, the concept of Shannon entropy is too rigid, so analysts prefer the more flexible concept of generalized entropy, which fulfills the first three Shannon-Khinchin axioms but not the fourth. These entropies include the Renyi and Tsallis entropies. In my talk I will show that generalized entropies are required to cope with the needs of time series analysis, in particular of symbolic representations with permutations.

## [01933] Fluid-structure interactions in Stokes flows

**Session Time & Room :**

01933 (1/3) : 1C (Aug.21, 13:20-15:00) @D403

01933 (2/3) : 1D (Aug.21, 15:30-17:10) @D403

01933 (3/3) : 1E (Aug.21, 17:40-19:20) @D403

**Type :** Proposal of Minisymposium

**Abstract :** The minisymposium focuses on computational methods for low (zero) Reynolds number flows, where viscous effects dominate. Due to the linearity of the fluid governing equations at zero Reynolds number, considerable progress in numerical methods has been made to understand the fluid-structure interactions at this small scale. This minisymposium will cover recent developments in numerical methods for modeling and simulating systems involving small immersed structures and suspensions of rigid and deformable particles, such as cilia, capsules, microorganisms, actin filaments in the cell cytoskeleton, catalytic colloids, electrolyte solutions in microfluidics or batteries, and others.

**Organizer(s) :** Aleksandar Donev, Yuan-Nan Young

**Classification :** 76-10, 76-00, 74F10, fluid-structure interactions, boundary integral methods, immersed boundary methods

**Minisymposium Program :**

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01933 (1/3) : 1C @D403 [Chair: Mike Miksis]

## [04825] Cross-stream migration of vesicles in vortical flows

**Format :** Online Talk on Zoom

**Author(s) :** Gokberk Kabacaoglu (Bilkent University )

**Abstract :** We use numerical simulations to systematically investigate the vesicle dynamics in two-dimensional (2D) Taylor-Green vortex flow in the absence of inertial forces. We study the effects of two parameters on the vesicle dynamics: the ratio of the interior fluid viscosity to that of the exterior one and the ratio of the shear forces on the vesicle to the membrane stiffness (characterized by the capillary number).

## [04962] Confinement effects on a suspension of squirmers

**Format :** Talk at Waseda University

**Author(s) :** Yuan Nan Young (New Jersey Institute of Technology)Bryan Quaife (Florida State University)Henry Shum (University of Waterloo)Sangwoo Shin (University at Buffalo)

**Abstract :** Using a model recently developed for the many-body hydrodynamics of amphiphilic JPs suspended in a viscous background flow (JFM, 941, 2022), we investigate how various swimming dynamics of squirmers that interact with the solvent through a hydrophobic potential (HP) may vary from tuning the hydrophobicity/hydrophilicity of the squirmers. In the absence of such HP, several configurations of squirmers are known to be stable for squirmers to swim together. We numerically investigate how HP may help stabilize/destabilize these configurations. These results are further compared with the Vicsek model for schooling and flocking of swimmers. We further investigate the effects of confinement and how active control of HP may be used for a cluster of swimmers to swim in specific fashions, indicating that the squirmers may actively change their surface properties so the collective of squirmers may swim in certain ways.

## [04477] Hydrodynamics and rheology of fluctuating, semiflexible, inextensible, and slender filaments in Stokes flow

**Format :** Talk at Waseda University

**Author(s) :** Aleksandar Donev (Courant Institute, New York University)

**Abstract :** Every animal cell is filled with a cytoskeleton, a dynamic gel made of inextensible filaments / bio-polymers, such as microtubules, actin filaments, and intermediate filaments, all suspended in a viscous fluid. Similar suspensions of elastic filaments or polymers are widely used in materials processing. Numerical simulation of such gels is challenging because the filament aspect ratios are very large.

We have recently developed new methods for rapidly computing the dynamics of non-Brownian and Brownian inextensible slender filaments in periodically-sheared Stokes flow. We apply our formulation to a permanently and dynamically cross-linked actin mesh in a background oscillatory shear flow. We find that nonlocal hydrodynamics can change the visco-elastic moduli by as much as 40% at certain frequencies, especially in partially bundled networks.

I will focus on accounting for bending thermal fluctuations of the filaments by first establishing a mathematical formulation and numerical methods for simulating the dynamics of stiff but not rigid Brownian fibers in Stokes flow. I will emphasize open questions for the community such as whether there is a continuum limit of the Brownian contribution to the stress tensor from the filaments.

## [04813] Numerical simulations of swimming with multiple bacterial flagella

**Format :** Talk at Waseda University

**Author(s) :** Henry Shum (University of Waterloo)Vahid Nourian (University of Waterloo)

**Abstract :** To understand some of the consequences of different morphologies of flagellated bacteria, we numerically simulate their swimming motion using a boundary element-regularized Stokeslet method. The flagella are modelled as discretized Kirchhoff rods. We apply our model to: (i) bacteria with a pulling flagellum in front and a pushing flagellum at the rear, and (ii) bacteria with three pushing flagella. Bacterial hook flexibility and flagellar placement are important considerations, especially near a no-slip wall.

01933 (2/3) : 1D @D403 [Chair: Yuan-Nan Young]

## [05143] A multiscale framework for rigid bodies in Stokes flow with applications to nanocellulose

**Format :** Talk at Waseda University

**Author(s) :** Anna Broms (KTH Royal Institute of Technology)Gusten Isfeldt (KTH Royal Institute of Technology)Mattias Sandberg (KTH Royal Institute of Technology)Jakob Wohlert (KTH Royal Institute of Technology)Fredrik Lundell (KTH Royal Institute of Technology)Anna-Karin Tornberg (KTH Royal Institute of Technology)

**Abstract :** The dynamics of rod-like nanocellulose crystals in an aqueous suspension is modelled with the rigid multiblob method for Stokes flow, with particle interactions from an accurate potential obtained from molecular dynamics data fed to a neural network. Tools to control the error from the hydrodynamic interactions and from discretising the overdamped Langevin equation, describing the Brownian motion of the particles, enable predictions of physical properties difficult to measure in the lab.

## [04881] Bounds on particle configurations in an active suspension

**Format :** Talk at Waseda University

**Author(s) :** Scott Weady (Flatiron Institute)

**Abstract :** We present bounds on orientational order parameters in the Doi-Saintillan-Shelley kinetic theory of active suspensions. Using the energy method, we show isotropic suspensions are nonlinearly stable for sufficiently low activity. A similar approach admits nontrivial bounds on time averages of order parameters for all levels of activity that are consistent with nonlinear simulations. This work highlights the organizing role of activity in particle suspensions and places precise limits on how organized such systems can be.

## [04858] Drag force on spherical particles trapped at a liquid interface

**Format :** Talk at Waseda University

**Author(s) :** Zhi Zhou (Northwestern University)Petia M Vlahovska (Northwestern University)Michael J Miksis (Northwestern University)

**Abstract :** Here we present a combined asymptotic and numerical investigation of the fluid motion past spherical particles attached to a deformable interface undergoing uniform creeping flows in the limit of small Capillary number and small deviation of the contact angle from 90 degrees. The drag and torque coefficients are computed as a function of the contact angle, the viscosity ratio, the Bond number, the slip coefficient along the particle surface, and the distance between two particles.

## [05148] Bacterial collective motion and spread in porous media

**Format :** Talk at Waseda University

**Author(s) :** Yasser Almoteri (New Jersey Institute of Technology)Enkeleida Lushi (New Jersey Institute of Technology)

**Abstract :** We investigate through modeling, analysis and nonlinear simulations, the motion of micro-swimmers in fluids with resistance, which approximates porous wet media. We use a continuum model to describe the

part\_2

dynamics of bacteria each performing run-and-tumble motions, coupled to the dynamics of the immersing fluid modeled by the Stokes-Brinkman equation with an added active stress. The linear stability of the uniform isotropic state reveals that the Brinkman resistance weakens or fully suppresses the chaotic motion of the bacterial suspension. Simulations of the full nonlinear PDE system confirm the analytical results. We discuss how the fluid resistance inhibits the spread of bacteria, and its interplay with auto-chemotactic interactions and food chasing give rise to non-trivial dynamics. Last, we discuss simulations of the coupled motion of many individually-traced micro-swimmers in Brinkman flows.

01933 (3/3) : 1E @D403 [Chair: Henry Shum]

### **[02866] Soft magnetic microrobots move more efficiently with a flat tire**

**Format :** Talk at Waseda University

**Author(s) :** Brennan Sprinkle (Colorado School of Mines)Yan Gao (Colorado School of Mines)David Marr (Colorado School of Mines)Ning Wu (Colorado School of Mines)

**Abstract :** I'll discuss the rolling of active Pickering emulsions - small droplets (~10-100 um) covered in smaller (~1um) active particles that can be rolled along a surface by an external, AC magnetic field. Curiously, these droplets roll much faster and more efficiently when they have a larger area of contact with the confining surface. I'll describe experiments done by collaborators to validate this behavior and numerical simulations that I developed to quantify it.

### **[05297] Bacterial swarming above surfaces with friction**

**Format :** Talk at Waseda University

**Author(s) :** Enkeleida Lushi (New Jersey Institute of Technology)

**Abstract :** We present a mathematical model and numerical simulations for the collective dynamics of swimming bacteria above surfaces with and without friction. The bacteria are modeled as self-propelling force-dipole ellipsoids that interact with each-other and the surface through hydrodynamics and direct collisions. The conditions for when the surface friction is sufficient to render an individual swimmer immobile are determined, as well as the swimmer density needed to collectively generate fluid flow disturbances that are strong enough to help regain mobility. Analysis of the characteristics of the emerging collective dynamics reveals a phase diagram of qualitatively distinct regimes for varying swimmer shape and population densities. Lastly, we compare our findings with recent experimental results of swarming *Bacillus subtilis* mutants.

## **[01935] Advances in Inverse Problems and Imaging**

**Session Time & Room :**

01935 (1/3) : 1E (Aug.21, 17:40-19:20) @G809

01935 (2/3) : 2C (Aug.22, 13:20-15:00) @G809

01935 (3/3) : 2D (Aug.22, 15:30-17:10) @G809

**Type :** Proposal of Minisymposium

**Abstract :** With the promotion by both mathematics itself and the practical requirements from engineering, the interest of researches on inverse problems and imaging, has been growing vigorously recent decades. The characteristic of the ill-posedness for inverse problems and imaging makes it hard to construct solutions. To overcome difficulties, various regularization techniques must be introduced which are closely related to many mathematical branches such as partial differential equations, differential geometry, numerical analysis, machine learning, image processing, functional analysis, optimizations and computer science. This minisymposium will bring together experts to discuss recent progresses in this area and related topics.

**Organizer(s) :** Gang Bao, Xiang Xu, Bo Zhang

**Classification :** 35R30, 49N45, 65N21

**Minisymposium Program :**

01935 (1/3) : 1E @G809 [Chair: Gang Bao]

part\_2

## [03733] Increasing stability in the linearized inverse Schrodinger potential problems

**Format :** Talk at Waseda University

**Author(s) :** Shuai Lu (Fudan University)

**Abstract :** Inverse Schrodinger potential problem concerns about the recovery of a potential function in the Schrodinger equation in a bounded domain through the DtN map. In this talk, we introduce the linearized DtN map, and prove a stability estimate with explicit dependence on wavenumbers. This is an increasing stability result, in the sense that the logarithmic stable term decays when wavenumber increases. The talk is based on joint works with Victor Isakov (Wichita), Mikko Salo (Jyvaskyla), Boxi Xu (SUFÉ) and Sen Zou (Fudan).

## [03422] High-order boundary integral equation solvers for layered-medium scattering problems

**Format :** Talk at Waseda University

**Author(s) :** Tao Yin (Chinese Academy of Sciences)

**Abstract :** This talk will present our recent works on the fast and highly accurate boundary integral equation (BIE) methods, including the windowed Green function (WGF) method and perfectly-matched-layer (PML) BIE method, for solving the acoustic and elastic wave scattering problems in both two- and three-dimensional layered-medium. 1) The WGF method utilizes the free-space fundamental solution to derive the BIEs on the whole unbounded surface which requires to be truncated in practical computing. Based on the solutions due to the scattering by flat surface, a correction strategy is introduced to ensure uniform accuracy for all incident angles. 2) For the half-space and two layered-medium case, the original scattering problem can be truncated onto a bounded domain by the PML. Assuming the vanishing of the scattered field on the PML boundary, BIEs on local defects are derived only in terms of using the PML-transformed free-space Green's function. For the considered two methods, a high-order Chebyshev-based rectangular-polar singular-integration solver is used in numerical implementation. Numerical experiments for both two- and three-dimensional problems are carried out to demonstrate the accuracy and efficiency of the proposed solvers. Potential applications to the inverse problems of reconstructing unbounded surfaces will also be discussed.

## [04333] An inverse boundary value problem for a nonlinear elastic wave equation

**Format :** Talk at Waseda University

**Author(s) :** Jian Zhai (Fudan University)

**Abstract :** We consider an inverse boundary value problem for a nonlinear model of elastic waves. We show that all the material parameters appearing in the equation can be uniquely determined from boundary measurements under certain geometric conditions. The proof is based on the construction of Gaussian beam solutions.

## [03434] Inverse random scattering problems for stochastic wave equations

**Format :** Talk at Waseda University

**Author(s) :** Jianliang Li (Hunan Normal University)Peijun Li (Purdue University)Xu Wang (Chinese Academy of Sciences)

**Abstract :** Inverse random scattering problems with a random source or potential will be introduced for time-harmonic wave equations. The unknown random source or potential is assumed to be a generalized isotropic Gaussian random field. With information of the data observed in a bounded domain, the strength of the random source or potential is shown to be uniquely determined by a single realization of the magnitude of the wave field averaged over the frequency band almost surely.

01935 (2/3) : 2C @G809 [Chair: Bo Zhang]

## [04564] An Inverse Problem for Nonlinear Time-dependent Schrodinger Equations with Partial Data

**Format :** Talk at Waseda University

**Author(s) :** Ting Zhou (Zhejiang University)Ru-Yu Lai (University of Minnesota)Xuezhu Lu (Northeastern University)

**Abstract :** In this talk, I will present some recent results on solving inverse boundary value problems for nonlinear PDEs, especially for a time-dependent Schrodinger equation with time-dependent potentials with partial boundary

part\_2

Dirichlet-to-Neumann map. After a higher order linearization step, the problem will be reduced to implementing special geometrical optics (GO) solutions to prove the uniqueness and stability of the reconstruction. This is a joint work with my PhD student Xuezhu Lu and Prof. Ru-Yu Lai.

## [04099] Inverse scattering problems with incomplete data

**Format :** Talk at Waseda University

**Author(s) :** Xiaodong Liu (Academy of Mathematics and Systems Science, Chinese Academy of Sciences)

**Abstract :** Inverse scattering problems aim to determine unknown scatterers with wave fields measured around the scatterers. However, from the practical point of views, we have only limited information, e.g., limited aperture data phaseless data and sparse data. In this talk, we introduce some data retrieval techniques and the applications in the inverse scattering problems. The theoretical and numerical methods for inverse scattering problems with multi-frequency spase measurements will also be mentioned.

## [03745] Imaging of penetrable locally rough surfaces from phaseless total-field data

**Format :** Talk at Waseda University

**Author(s) :** Haiwen Zhang (Academy of Mathematics and Systems Science, Chinese Academy of Sciences)Long Li (Academy of Mathematics and Systems Science, Chinese Academy of Sciences)Jiansheng Yang (Peking University)Bo Zhang (Academy of Mathematics and Systems Science, Chinese Academy of Sciences)

**Abstract :** This talk is concerned with inverse scattering by a two-layered medium with a locally rough interface in 2D. We propose a direct imaging method to reconstruct the penetrable locally rough surface from phaseless total-field data. The theoretical analysis is mainly based on the results in our recent work (L. Li, J. Yang, B. Zhang and H. Zhang, arXiv:2208.00456) on the uniform far-field asymptotics of the scattered field for acoustic scattering in a two-layered medium.

## [04075] A new approach to an inverse source problem for the wave equation

**Format :** Talk at Waseda University

**Author(s) :** Haibing Wang (Southeast University)

**Abstract :** Consider an inverse problem of reconstructing a source term from boundary measurements for the wave equation. We propose a novel approach to recover the unknown source through measuring the wave fields after injecting small particles, enjoying a high contrast, into the medium. For this purpose, we first derive the asymptotic expansion of the wave field, based on the time-domain Lippmann-Schwinger equation. The dominant term in the asymptotic expansion is expressed as an infinite series in terms of the eigenvalues of the Newtonian operator (for the pure Laplacian). Such expansions are useful under a certain scale between the size of the particles and their contrast. Second, we observe that the relevant eigenvalues appearing in the expansion have non-zero averaged eigenfunctions. By introducing a Riesz basis, we reconstruct the wave field, generated before injecting the particles, on the center of the particles. Finally, from these last fields, we reconstruct the source term. A significant advantage of our approach is that we only need the measurements for a single point away from the support of the source. This is a joint work with Prof. Mourad Sini from RICAM.

01935 (3/3) : 2D @G809 [Chair: Xiang Xu]

## [04288] Recovering an infinite rough surface by acoustic measurements

**Format :** Talk at Waseda University

**Author(s) :** Jiaqing Yang (Xi'an Jiaotong University)

**Abstract :** In this talk, I will report some recent advances on inverse scattering by rough surfaces, where new uniqueness results and inversion algorithms will be presented to recover the shape and location of the rough surface from the near-field measurements associated with incident point sources. Moreover, several numerical examples will be provided to illustrate the effectiveness of the algorithms.

## [03405] Uniqueness on recovering coefficients from localized Dirichlet-to-Neumann map for piecewise homogeneous piezoelectricity

**Format :** Talk at Waseda University

**Author(s) :** Xiang Xu (Zhejiang University)

**Abstract :** In this talk, we present an inverse problem on determining coefficients of piecewise homogeneous piezoelectric equations from a localized Dirichlet-to-Neumann map on partial boundaries. Assume the bounded domain can be divided into finite subdomains, in which the unknown coefficients including the anisotropic elastic tensor, the piezoelectric tensor, and the dielectric tensor are constants. Two different cases are considered: the subdomains are either known and Lipschitz or unknown and subanalytic. For both cases, the unknown coefficients can be uniquely determined from a given localized Dirichlet-to-Neumann map.

## [01952] Mathematical models of morphogenesis and morphological deformation in living organisms

**Session Time & Room :** 4E (Aug.24, 17:40-19:20) @A512

**Type :** Proposal of Minisymposium

**Abstract :** The objective of our proposal is to present recent development of mathematical theory of morphogenesis and morphological deformation in living organisms. The topics are dynamics of endothelial cells in angiogenesis, i.e., the formation of networks of blood vessels, morphogenetic processes of organs, homeostasis of precursor cells in the brain and the genesis of a glioma and sol-gel transition of teleost muscular proteins. In each talk, both recent experimental results and the mathematical models, which can be used for the analysis of them, are presented.

**Organizer(s) :** Tetsuji Tokihiro

**Classification :** 92-10, 92C15, 92C37

**Minisymposium Program :**

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01952 (1/1) : 4E @A512 [Chair: Tetsuji Tokihiro]

## [02830] A kinetic model for sol-gel transition of teleost muscular proteins

**Format :** Talk at Waseda University

**Author(s) :** Yuri Kominami (The University of Tokyo)

**Abstract :** Various enzymatic reactions have a critical role in control of cellular function in living tissue. The enzymes can be activated in the tissue after organismal death and cause post-mortem changes. The enzymes delivered from animal tissue are also activated during food processing and affect product attributes. In this talk, the enzymatic reactions during sol-gel transition of teleost muscular proteins will be addressed and a kinetic model will be discussed.

## [03680] Mathematical model for dynamics of endothelial cells in sprouting angiogenesis

**Format :** Talk at Waseda University

**Author(s) :** Tatsuya Hayashi (Yamato University)

**Abstract :** Angiogenesis is a morphogenic process that involves the emergence of new blood vessels from an existing vascular network. We propose a mathematical model based on the characteristic movements of endothelial cells in angiogenesis. In this presentation, we show that our model is able to reproduce the coordinated linear and rotational movements observed in a two-cell state, as well as angiogenic morphogenesis and the effects of cell adhesion molecules in a multicellular simulation.

## [04407] Measurement and mathematical analysis of organ morphogenetic processes

**Format :** Talk at Waseda University

**Author(s) :** Yoshihiro Morishita (RIKEN Center for Biosystems Dynamics Research)

**Abstract :** The physical processes that govern the formation of almost all organs, namely, collective cell motion and tissue-level deformation, remain largely unknown. However, recent advances in microscopy have enabled the measurement and quantification of these dynamics. In this study, we investigate the early development of the forebrain and heart and present our findings on the morphogenetic rules that underlie their formation, based on our analysis of the measured morphogenetic dynamics.

## [03395] A mathematical model for the evolution of low-grade gliomas before and after radiotherapy

**Format :** Talk at Waseda University

**Author(s) :** Mathilde Badoual (Paris Cité University)Leo Adenis (CNRS)Stephane Plaszczynski (CNRS)Jean-Eric Campagne (CNRS)Basile Grammaticos (CNRS)Johan Pallud (Sainte-Anne Hospital)

**Abstract :** Diffuse low-grade gliomas are slowly growing tumors that mainly affect adults around 40 years old and are incurable. After tens of years, they transform inexorably into more aggressive forms, jeopardizing the patient's life. Mathematical modeling could help clinicians to have a better understanding of the underlying biological process involved in the evolution of these tumors and their response to treatments. We present here a model of evolution of these tumors, based on a PDE that describes the evolution of the cell density and the effect of radiotherapy. This model is used to fit clinical data (MRI scans), and to predict the regrowth time after radiotherapy.

## [01996] Control and inverse problems on waves, oscillations and flows

**Session Time & Room :**

01996 (1/3) : 2E (Aug.22, 17:40-19:20) @G809

01996 (2/3) : 3C (Aug.23, 13:20-15:00) @G809

01996 (3/3) : 3D (Aug.23, 15:30-17:10) @G809

**Type :** Proposal of Minisymposium

**Abstract :** The identification of unknown ingredients in wave, oscillation and flow phenomena governed by evolutionary PDEs from observational data is a central challenge in a variety of areas of science and engineering. This mini-symposium aims at gathering together international scientific researchers to share the latest progress on the related control and inverse problems. It provides a platform to discuss recent developments and emerging challenges, which include but are not limited to

1. Stability and controllability for inverse parabolic and hyperbolic problems;
2. Uniqueness of inverse problems for subdiffusion and viscoelasticity;
3. Data-driven inversion methods and optimal control;
4. Related numerical schemes for reconstruction.

**Organizer(s) :** Hiromichi Itou, Atsushi Kawamoto, Yikan Liu, Hisashi Morioka

**Classification :** 35R30, 35Q93, 35R11, 65M30

**Minisymposium Program :**

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01996 (1/3) : 2E @G809 [Chair: Yikan Liu]

## [03795] Recovery in vivo viscoelasticity from elastography measured data

**Format :** Talk at Waseda University

**Author(s) :** Yu Jiang (Shanghai University of Finance and Economics)

**Abstract :** This talk will briefly describe how to solve the inverse problem of recovering in vivo viscoelasticity from elastography (magnetic resonance elastography, ultrasound elastography) measurements. To solve it robustly, one need to have a proper partial differential equation model to describe the wave motion inside living body. And based on this PDE model and given interior measurements, theoretical and numerical inverse analyzes need to be performed. As the PDE model, we start with a dynamic viscoelastic model and several simplified models are given. For inversion analysis, we give several practical numerical inversion methods to identify viscoelasticity, such as regularized numerical differentiation method etc.

## [03880] Acousto-electric tomography imaging model and algorithm based on two-point gradient method

**Format :** Talk at Waseda University

**Author(s) :** Min Zhong (School of Mathematics, Southeast University )

**Abstract :** We study the numerical reconstruction problem in acousto-electric tomography of recovering the conductivity distribution in a bounded domain from interior power density data. We propose a numerical method for recovering discontinuous conductivity distributions, by utilizing the two point gradient method, the piecewise constant conductivity can be efficiently reconstructed. Extensive numerical experiments are presented to illustrate the feasibility of the proposed approach.

## [04269] Numerical method for unique continuation of elliptic equations and applications

**Format :** Talk at Waseda University

**Author(s) :** Yu Chen (Shanghai University of Finance and Economics)Jin Cheng (Fudan University)

**Abstract :** Numerical method for unique continuation of elliptic equations is related to information reconstruction from interior local measurements. The conditional stability of unique continuation along analytic sub-manifolds in three dimensions will be provided. A stable numerical algorithm is constructed based on Tikhonov regularization according to the conditional stability, in order to deal with the ill-posedness. The evaluation of reliable region of a reconstruction and potential applications of the present method in atmospheric flows will be discussed.

## [04089] Reconstruction of piecewise smooth diffusion coefficient and initial value with adaptive regularization

**Format :** Talk at Waseda University

**Author(s) :** Shuli CHEN (Hokkaido University)Haibing Wang (Southeast University)

**Abstract :** This talk will present an inverse problem of simultaneously reconstructing the piecewise smooth diffusion coefficient and initial value in a diffusion equation from extra measurements. The inverse problem is transformed into solving an optimization problem with a switchable regularization to simultaneously preserve multiple properties of unknown functions. The existence, stability and consistency result are rigorously analyzed by introducing a domain index. Then, we decompose the optimization problem into a SOLVE-MARK-REFINE-looping scheme and develop an adaptive iterative algorithm. Finally, we present several numerical examples to show the validity of the proposed algorithm.

01996 (2/3) : 3C @G809 [Chair: Hiromichi Itou]

## [04229] Inverse problems for the Duffing equation in pediatrics

**Format :** Talk at Waseda University

**Author(s) :** Manabu Machida (Hamamatsu University School of Medicine)

**Abstract :** The prognostic prediction of the neonatal hypoxic-ischemic encephalopathy (HIE) has been tried with near-infrared spectroscopy. In this talk, the Duffing equation is proposed as a model which governs the time-evolution of the cerebral blood volume. We will consider an inverse problem of determining coefficients and initial values of the equation.

## [04402] Unique determination of source and Robin coefficient in fractional diffusion equation

**Format :** Talk at Waseda University

**Author(s) :** Zhiyuan Li (Ningbo University)Daijun Jiang (Central Central China Normal University)China Normal University)

**Abstract :** In this talk, we consider an inverse problem of simultaneously determining the spatially dependent source term and the Robin boundary coefficient in a time fractional diffusion equation, with the aid of extra measurement data at a subdomain near the accessible boundary. Firstly, the spatially varying source is uniquely determined in view of the unique continuation principle and Duhamel principle for the fractional diffusion equation. The Hopf lemma for a homogeneous time-fractional diffusion equation is proved and then used to prove the uniqueness of recovering the Robin boundary coefficient.

## [05327] Fine-tuning neural-operator architectures for training and generalization

**Format :** Talk at Waseda University

**Author(s) :** Takashi Furuya (Shimane University)

**Abstract :** We investigate the generalization error of Neural Operators (NOs), which aim to approximate the forward operator in PDEs, and propose modifications of NOs, referred to as  $s\text{NO} + \varepsilon$ . We establish generalization error bounds for both NOs and  $s\text{NO} + \varepsilon$ , and we observe that our bound is sharper than that for NOs. Additionally, our experiments, particularly the wave equation experiment, demonstrate that our proposed network exhibits remarkable generalization capabilities, whereas NOs perform poorly in out-of-distribution scenarios.

## [03684] Reconstruction of location for a single point target in time-domain fluorescence diffuse optical tomography

**Format :** Talk at Waseda University

**Author(s) :** Junyoung Eom Gen Nakamura (Hokkaido University)Goro Nishimura (Hokkaido University)Chunlong Sun (Nanjing University of Aeronautics and Astronautics)

**Abstract :** The time-domain fluorescence diffuse optical tomography (FDOT) problem is to recover the distribution of fluorophores in biological tissue from the time-domain measurement on the boundary. The measurement is conducted by several pairs (S-D pairs) of a point source and a point detector. In this paper, we identify the location of the distribution of fluorophores over a point, refer as a point target. We first express a solution for the forward problem in a dimensionless form and consider its asymptotic expansion. Then, we theoretically investigate the minimal number of S-D pairs to determine the point target location, analyzing the sensitivity matrix. Finally, we numerically verify the invertibility of the matrix and demonstrate the local solvability for locating well-separated multiple point targets.

01996 (3/3) : 3D @G809 [Chair: Atsushi Kawamoto]

## [05416] STABILITY ESTIMATES FOR AN INVERSE PROBLEM FOR SCHRODINGER OPERATORS AT HIGH FREQUENCIES FROM ARBITRARY PARTIAL BOUNDARY MEASUREMENTS

**Format :** Online Talk on Zoom

**Author(s) :** Ganghua Yuan Xiaomeng Zhao (Northeast Normal University)

**Abstract :** In this talk, we consider the partial data inverse boundary value problem for the Schrodinger operator at a high frequency in a bounded domain in  $\mathbb{R}^n$ ,  $n \geq 3$ . Assuming that the potential is known in a neighborhood of the boundary, we obtain the logarithmic stability when both Dirichlet and Neumann data are taken on arbitrary open subsets of the boundary . We used a method combining the CGO solution, Runge approximation and Carleman estimate.

## [04623] Carleman estimates and some inverse problems for the coupled quantitative thermoacoustic equations

**Format :** Online Talk on Zoom

**Author(s) :** Michel Cristofol (Aix-Marseille Université) Shumin Li (University of Science and Technology of China) Yunxia Shang (Shanghai Normal University)

**Abstract :** We consider the determination of a coefficient or the source term in a strong coupled quantitative thermoacoustic system of equations. For this purpose, we establish a Carleman estimate for the coupled quantitative thermoacoustic equations. Applying this Carleman estimate, we prove stability estimates of Hölder type for inverse problems involving the observation of only one component: the temperature or the pressure.

## [02703] Numerical reconstruction of the spatially dependent source term in a time-fractional diffusion equation

**Author(s) :** Daijun Jiang (Central China Normal University)

**Abstract :** In this talk, we are concerned with the analysis on the numerical reconstruction of the spatial component in the source term of a time-fractional diffusion equation. This ill-posed problem is solved through a stabilized nonlinear minimization system by an appropriately selected Tikhonov regularization. The existence and the stability of the optimization system are demonstrated. The nonlinear optimization problem is approximated by a fully discrete scheme, whose convergence is established under a novel result verified in this study that the H<sub>1</sub>-norm of the solution to the discrete forward system is uniformly bounded. The iterative thresholding algorithm is proposed to solve the discrete minimization, and several numerical experiments are presented to show the efficiency and the accuracy of the algorithm.

## [04572] Unique continuation for wave equations in asymptotically anti-de Sitter spaces

**Format :** Talk at Waseda University

**Author(s) :** Hiroshi Takase (Kyushu University)

**Abstract :** An asymptotic anti-de Sitter space is a Lorentzian manifold with a Lorentz metric diverging at the boundary of the manifold. It is also used as a model of outer space, and in particular, the problem of determining the inner structure from the data at the boundary has attracted attention in theoretical physics as AdS/CFT correspondence. The wave equation in this space is a degenerate equation. In this talk, I will present results on the fundamental property of unique continuation for this wave equation.

# [02012] Splitting Optimization: Theory, Methodology and Application

**Session Time & Room :**

02012 (1/4) : 2E (Aug.22, 17:40-19:20) @A207

02012 (2/4) : 3C (Aug.23, 13:20-15:00) @A207

02012 (3/4) : 3D (Aug.23, 15:30-17:10) @A207

02012 (4/4) : 3E (Aug.23, 17:40-19:20) @A207

**Type :** Proposal of Minisymposium

**Abstract :** With the development of artificial intelligence, big data and other applications, large-scale optimization problems have received more and more attention. The advantage of the splitting method is to make use of the problem structure to reasonably disassemble the large-scale optimization problem into a series of subproblems, and to solve the large-scale optimization problem efficiently through the "decomposition-integration" architecture. This minisymposium introduces splitting optimization through a series of reports, including theories, methods, and applications.

**Organizer(s) :** Deren Han, Xingju Cai, Xiangfeng Wang

**Classification :** 90C30, 65K05

**Minisymposium Program :**

02012 (1/4) : 2E @A207 [Chair: Xingju Cai]

## [02878] Decentralized Entropic Optimal Transport for Privacy-preserving Distributed Distribution Comparison

**Format :** Talk at Waseda University

**Author(s) :** Xiangfeng Wang (East China Normal University)

**Abstract :** Privacy-preserving distributed distribution comparison measures the distance between the distributions whose data are scattered across different agents in a distributed system and cannot be shared among the agents. In this study, we propose a novel decentralized entropic optimal transport (EOT) method, which provides a privacy-preserving and communication-efficient solution to this problem with theoretical guarantees. In particular, we design a mini-batch randomized block-coordinate descent (MRBCD) scheme to optimize the decentralized EOT distance in its dual form. The dual variables are scattered across different agents and updated locally and iteratively with limited communications among partial agents. The kernel matrix involved in the gradients of the dual variables is estimated by a distributed kernel approximation method, and each agent only needs to approximate and store a sub-kernel matrix by one-shot communication and without sharing raw data. We analyze our method's communication complexity and provide a theoretical bound for the approximation error caused by the convergence error, the approximated kernel, and the mismatch between the storage and communication protocols. Experiments on synthetic data and real-world distributed domain adaptation tasks demonstrate the effectiveness of our method.

## [02881] An alternative extrapolation scheme of PDHGM for saddle point problem with nonlinear function

**Format :** Talk at Waseda University

**Author(s) :** Wenxing Zhang (University of Electronic Science and Technology of China)

**Abstract :** Primal-dual hybrid gradient method (PDHG) is a canonical and popular prototype for solving saddle point problem (SPP). However, the nonlinear coupling term in SPP excludes the application of PDHG on far-reaching real-world problems. In this talk, we devise a variant iterative scheme for solving SPP with nonlinear function by exerting an alternative extrapolation procedure. Under the metrically regular assumption on KKT mapping, we simplify the local convergence of the proposed method on contractive perspective. Numerical simulations on a PDE-constrained nonlinear inverse problem and parametric blind deconvolution demonstrate the compelling performance of the proposed method.

## [02882] A balanced Douglas-Rachford splitting algorithm for convex minimization

**Format :** Talk at Waseda University

**Author(s) :** Xingju Cai (Nanjing Normal University)

**Abstract :** The Douglas-Rachford algorithm is a classical and effective splitting method to solve the inclusion problems. Recently, an adaptive Douglas-Rachford splitting algorithm is proposed for the monotone inclusion, which allow one operator be weakly monotone. We apply the idea of adaptive Douglas-Rachford splitting method (ADRSRM) to differentiable convex optimization problems with abstract constraints, and more attractive results can be obtained for the convex optimization problem. We propose accurate and inaccurate versions of the algorithm respectively, and prove the global convergence of the algorithms. We extend these results to two separable convex optimization problems with linear constraints. In numerical experiments, we compare our algorithms with other commonly used algorithms and the results verify the effectiveness of our algorithms.

## [02904] A projection-like method for quasimonotone variational inequalities without Lipschitz continuity

**Format :** Talk at Waseda University

**Author(s) :** Lingling Xu (Nanjing Normal University)Xiaoxi Jia (Institute of Mathematics, University of Würzburg,)

**Abstract :** For most projection methods, the operator of a variational inequality problem is assumed to be monotone (or pseudomonotone) and Lipschitz continuous. In this paper, we present a projection-like method to solve quasimonotone variational inequality problems without Lipschitz continuity. Under some mild assumptions, we prove that the sequence generated by the proposed algorithm converges to a solution. Numerical experiments are provided to show the effectiveness of the method.

02012 (2/4) : 3C @A207 [Chair: Deren Han]

## [02918] A trust-region-based splitting method for linear constrained programs

**Format :** Talk at Waseda University

**Author(s) :** Deren Han (Beihang University)

**Abstract :** The augmented Lagrangian based splitting methods have found more and more applications in scientific and engineering computation, such as compressive sensing, covariance selection, image processing and transportation research. One of the basic difficulties in such algorithms is the selection of the parameter in the augmented Lagrangian function, a larger one may make the primal progress too small while a small one may slow down the dual progress. To overcome this difficulty, in this paper, we propose to solve the splitting subproblems in a trust-region manner, and the radius can be adjusted smartly. Under the same mild conditions as those for classical augmented Lagrangian based splitting methods, we prove the global convergence of the proposed algorithm. Moreover, the  $\mathcal{O}(1/\epsilon)$  convergence rate is also analyzed in an ergodic sense. We present some preliminary numerical experiments on medical image recovery and traffic assignment, which show that the trust-region-based splitting method is efficient and promising.

## [02995] A Decentralized Second-Order Multiplier Algorithm with Quasi-Newton Tracking

**Format :** Talk at Waseda University

**Author(s) :** Liping Wang (Nanjing University of Aeronautics and Astronautics)

**Abstract :** In this talk, we consider a decentralized optimization problem of minimizing a finite sum of strongly convex and twice continuously differentiable functions over a fixed connected undirected network. We propose a fully decentralized second-order multiplier algorithm (DSOM) where second-order information are approximated by simple algebraic calculations and at most matrix-vector products. It is the first work to study the second-order multiplier method in decentralized optimization which is equivalent to the primal-dual method with twice primal quasi-Newton steps and once dual BB step per iteration. Additionally, in DSOM the local direction on each node asymptotically approximates the global quasi-Newton direction. Under some mild assumptions, the proposed algorithm is illustrated to have global linear convergence rate. Numerical results are also reported for verifying its effectiveness.

## [03066] Tight Convergence Rate in Subgradient Norm of the Proximal Point Algorithm

**Format :** Talk at Waseda University

**Author(s) :** Guoyong Gu (Nanjing University) Junfeng Yang (Nanjing University)

**Abstract :** Proximal point algorithm has found many applications, and it has been playing fundamental roles in the understanding, design, and analysis of many first-order methods. In this paper, we derive the tight convergence rate in subgradient norm of the proximal point algorithm, which was conjectured by Taylor, Hendrickx and Glineur [SIAM J. Optim., 27 (2017), pp. 1283–1313].

## [03073] A fast PIRNN algorithm for nonconvex low-rank matrix minimization problems

**Format :** Talk at Waseda University

**Author(s) :** Zhili Ge (Nanjing Normal University of Special Education)

**Abstract :** In this paper, we propose a fast PIRNN algorithm with extrapolation for solving a class of nonconvex low-rank matrix minimization problems. The proposed method incorporates two different extrapolation steps with respect to the previous iterations into the backward proximal step and the forward gradient step of the classic proximal iteratively reweighted method. We prove that the proposed method generates a convergent subsequence under general parameter constraints, and that any limit point is a stationary point of the problem. Furthermore, we prove that if the objective function satisfies the KL property, the algorithm is globally convergent to a stationary point of the considered problem. Finally, we perform numerical experiments on a practical matrix completion problem with both synthetic and real data, the results of which demonstrate the efficiency and superior performance of the proposed algorithm.

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02012 (3/4) : 3D @A207 [Chair: Xinxin Li]

## [03085] Gradient methods using Householder transformation with application to hypergraph partitioning

**Format :** Talk at Waseda University

**Author(s) :** Xin Zhang ( Suzhou University)Jingya Chang (Guangdong University of Technology)Zhili Ge (, Nanjing Normal University of Special Education)Zhou Sheng (Anhui University of Technology)

**Abstract :** In this paper, we propose a constraint preserving algorithm for the smallest Z-eigenpair of the compact Laplacian tensor of an even-uniform hypergraph, where Householder transform is employed and a family of modified conjugate directions with sufficient descent is determined. Besides, we prove that there exists a positive step size in the new constraint preserving update scheme such that the Wolfe conditions hold. Based on these properties, we prove the convergence of the new algorithm. Furthermore, we apply our algorithm to the hypergraph partitioning and image segmentation, numerical results are reported to illustrate the efficiency of the proposed algorithm.

## [03102] Solving saddle point problems: a landscape of primal-dual algorithm with larger stepsizes

**Format :** Talk at Waseda University

**Author(s) :** Fan Jiang (Nanjing University of Information Science and Technology)Hongjin He (Ningbo University)Zhiyuan Zhang (Xiamen University)

**Abstract :** We consider a class of saddle point problems frequently arising in the areas of image processing and machine learning. In this paper, we propose a simple primal-dual algorithm, which embeds a general proximal term induced with a positive definite matrix into one subproblem. It is remarkable that our algorithm enjoys larger stepsizes than many existing state-of-the-art primal-dual-like algorithms due to our relaxed convergence-guaranteeing condition. Moreover, our algorithm includes the well-known primal-dual hybrid gradient method as its special case, while it is also of possible benefit to deriving partially linearized primal-dual algorithms. Finally, we show that our algorithm is able to deal with multi-block separable saddle point problems. In particular, an application to a multi-block separable minimization problem with linear constraints yields a parallel algorithm. Some computational results sufficiently support the promising improvement brought by our relaxed requirement.

## [03200] Inexact variable metric proximal incremental aggregated gradient algorithm for nonconvex nonsmooth optimization problem

**Author(s) :** zehui Jia (Nanjing University of Information Science and Technology)junru Hou (Nanjing University of Information Science and Technology)xingju Cai (Nanjing Normal University)

**Abstract :** This paper focuses on the problem that minimizing the sum of a nonconvex smooth function and a nonsmooth convex function, in which the smooth term is in the form of finite sum. In order to solve the problem efficiently, we introduce the idea of incremental aggregation and two different inexact criterions to the variable metric proximal gradient (VMPG) algorithms, and then propose the inexact variable metric proximal incremental aggregated gradient (iVMPAG) algorithms, i.e., iVMPAG-I, iVMPAG-II. Under the Kurdyka-Łojasiewicz (KL) property, we show the global convergence of iVMPAG-I and iVMPAG -II. When the Łojasiewicz exponent is known, we can prove the convergence rate of iVMPAG-I with respect to the objective function value and the convergence rate of iVMPAG-II with respect to the iterative sequence. Note that, for the convergence analysis of iVMPAG-I, a critical tool is introduced, i.e., the incremental aggregated forward-backward (FB) envelope, which is a continuously differential function and can cover the FB envelope as a special case. Based on this tool, we define a continuously differentiable surrogate function, which equals to the value of the objective function at the stationary point. Finally, we present the efficiency of the iVMPAG method for large-scaled image restoration problem.

## [03253] A Restricted Dual PRSM for a Strengthened DNN Relaxation for QAP

**Format :** Talk at Waseda University

**Author(s) :** Naomi Graham (University of British Columbia)Hao Hu (Clemson University)Jiyoung Im (University of Waterloo)Xinxin Li (Jilin University)Henry Wolkowicz (University of Waterloo)

**Abstract :** Splitting methods in optimization arise when one can divide an optimization problem into two or more simpler subproblems. They have proven particularly successful for relaxations of problems involving discrete variables. We revisit and strengthen splitting methods for solving doubly nonnegative, DNN, relaxations of the particularly difficult, NP-hard quadratic assignment problem, QAP. We use a modified restricted contractive splitting method, rPRSM, approach. In particular, we show how to exploit redundant constraints in the subproblems. Our strengthened bounds exploit these new subproblems, as well as new dual multiplier estimates, to improve on the bounds and convergence results in the literature.

## [02014] High-order numerical methods: recent development and applications

**Session Time & Room :**

02014 (1/4) : 1C (Aug.21, 13:20-15:00) @E709

02014 (2/4) : 1D (Aug.21, 15:30-17:10) @E709

02014 (3/4) : 1E (Aug.21, 17:40-19:20) @E709

02014 (4/4) : 2C (Aug.22, 13:20-15:00) @E709

**Type :** Proposal of Minisymposium

**Abstract :** Over the last few years, high-order numerical methods have found their way into the mainstream of computational sciences and are now being successfully applied in almost all areas of natural sciences and engineering. The aim of this minisymposium is to present the most recent developments in the design and theoretical analysis of high-order numerical methods, and to discuss relevant issues related to the practical implementation and applications of these methods. Topics include: theoretical aspects and numerical analysis of high-order numerical methods, non-linear problems, and applications.

**Organizer(s) :** Qi Tao, Yan Xu, Xinghui Zhong

**Classification :** 65MXX, 65NXX

**Minisymposium Program :**

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02014 (1/4) : 1C @E709 [Chair: Yan XU]

## [03002] High-order Structure-Preserving Schemes for Special Relativistic Hydrodynamics

**Format :** Talk at Waseda University

**Author(s) :** Huazhong Tang (Nanchang Hangkong University and Peking University)

**Abstract :** Abstract: This talk mainly reviews two high-order accurate structure-preserving finite difference schemes for the special relativistic hydrodynamics (RHD). The first is the physical-constraints-preserving (PCP) scheme, which preserves the positivity of the rest-mass density and the pressure and the bounds of the fluid velocity and is built on the local Lax-Friedrichs (LxF) splitting, the WENO reconstruction, the PCP flux limiter, and the high-order strong stability preserving time discretization. The key to developing such scheme is to prove the convexity and other properties of the admissible state set and to discover a concave function with respect to the conservative vector. The second is the entropy stable (ES) scheme, whose semi-discrete version satisfies the entropy inequality. The key is to technically construct the affordable entropy conservative (EC) flux of the semi-discrete second-order accurate EC schemes satisfying the semi-discrete entropy equality for the found convex entropy pair. As soon as the EC flux is derived, the dissipation term can be added to give the semi-discrete ES schemes satisfying the semi-discrete entropy inequality. The WENO reconstruction for the scaled entropy variables and the previous time discretization are implemented to obtain the fully-discrete high-order “ES” schemes. The performance of the proposed schemes has been demonstrated by numerical experiments. By the way, we also briefly review other relative works on the structure-preserving schemes for the special RHDs. Those works have been further to the general equation of state and the special relativistic magnetohydrodynamics etc., see our papers listed below for details.

References

1. Wu, K.L. and Tang, H.Z., “High-order accurate physical-constraints-preserving finite difference WENO schemes for special relativistic hydrodynamics”, J. Comput. Phys., Vol. 298, 2015, pp. 539-564.
2. Wu, K.L. and Tang, H.Z., “Physical-constraints-preserving central discontinuous Galerkin methods for special relativistic hydrodynamics with a general equation of state”, Astrophys. J. Suppl. ser., Vol. 228, 2017, 3.
3. Wu, K.L. and Tang, H.Z., “Admissible states and physical constraints preserving numerical schemes for special relativistic magnetohydrodynamics”, Math. Mod. and Meth. Appl. Sci., Vol. 27, 2017, pp. 1871-1928.

4. Wu, K.L. and Tang, H.Z., "On physical-constraints-preserving schemes for special relativistic magnetohydrodynamics with a general equation of state", Z. Angew. Math. Phys., Vol. 69, 2018, 84.
5. Ling, D., Duan, J.M. and Tang, H.Z., "Physical-constraints-preserving Lagrangian finite volume schemes for one- and two-dimensional special relativistic hydrodynamics", J. Comput. Phys., Vol. 396, 2019, pp. 507-543.
6. Ling, D. and Tang, H.Z., "Genuinely multidimensional physical-constraints-preserving finite volume schemes for the special relativistic hydrodynamics", submitted to Commun. Comput. Phys., March 4, 2023. arXiv: 2303.02686.
7. Duan, J.M. and Tang, H.Z., "High-order accurate entropy stable finite difference schemes for one- and two-dimensional special relativistic hydrodynamics", Adv. Appl. Math. Mech., Vol. 12, 2020, pp. 1-29.
8. Duan, J.M. and Tang, H.Z., "High-order accurate entropy stable nodal discontinuous Galerkin schemes for the ideal special relativistic magnetohydrodynamics", J. Comput. Phys., Vol. 421, 2020, 109731.
9. Duan, J.M. and Tang, H.Z., "Entropy stable adaptive moving mesh schemes for 2D and 3D special relativistic hydrodynamics", J. Comput. Phys., Vol. 426, 2021, 109949.

## [03400] High order entropy stable and positivity-preserving discontinuous Galerkin method for the nonlocal electron heat transport model

**Format :** Talk at Waseda University

**Author(s) :** Juan Cheng (Institute of Applied Physics and Computational Mathematics)

**Abstract :** The nonlocal electron heat transport model in laser heated plasmas plays a crucial role in inertial confinement fusion (ICF), and it is important to solve it numerically in an accurate and robust way. In this talk, we develop a class of high-order entropy stable discontinuous Galerkin methods for the nonlocal electron heat transport model. We further design our DG scheme to have the positivity-preserving property, which is shown, by a computer-aided proof, to have no extra time step constraint than that required by L2 stability. Numerical examples are given to verify the high-order accuracy and positivity-preserving properties of our scheme. By comparing the local and nonlocal electron heat transport models, we also observe more physical phenomena such as the flux reduction and the preheat effect from the nonlocal model.

## [02764] A new cut-cell interface treating method for compressible multi-medium flow

**Format :** Talk at Waseda University

**Author(s) :** Chunwu Wang (Nanjing University of Aeronautics and Astronautics)

**Abstract :** In this work, a conservative sharp interface treating method is proposed for solving compressible multi-medium flow based on the cut-cell method. To overcome the small cell problem, which causes standard explicit scheme unstable, the most common approach is generating interface cells by merging small cut cells with their neighbors. We present a new and simple way to construct interface cells. Rather than considering various complex cell merging cases, we select some Cartesian cell nodes near the interface, and then connect these nodes to form the interface cells. Meanwhile, at the edges of the cell coinciding with the interface, the numerical fluxes are obtained by solving the local Riemann problem, thus the conservation of the flow variables is effectively maintained. Several numerical experiments indicate that our proposed method can capture the shock wave and material interface accurately and sharply, as well as being stable even for problems with significant density and pressure gradients.

## [02690] A hybrid WENO scheme for steady Euler equations in curved geometries on Cartesian grids

**Format :** Talk at Waseda University

**Author(s) :** Yifei Wan (University of Science and Technology of China)Yinhua Xia (University of Science and Technology of China)

**Abstract :** For steady Euler equations in complex boundary domains, high-order shock-capturing schemes usually suffer not only from the difficulty of steady-state convergence but also from the problem of dealing with physical boundaries on Cartesian grids to achieve uniform high-order accuracy. In this work, we utilize a fifth-order finite difference hybrid WENO scheme to simulate steady Euler equations, and the same fifth-order WENO extrapolation methods are developed to handle the curved boundary. The values of the ghost points outside the physical boundary can be obtained by applying WENO extrapolation near the boundary, involving normal derivatives acquired by the simplified inverse Lax-Wendroff procedure. Both equivalent expressions involving curvature and numerical differentiation are utilized to transform the tangential derivatives along the curved solid wall boundary. This hybrid WENO scheme is robust for steady-state convergence and maintains high-order accuracy in the smooth region even with the solid wall boundary condition. Besides, the essentially non-oscillation property is achieved.

The numerical spectral analysis also shows that this hybrid WENO scheme possesses low dispersion and dissipation errors. Numerical examples are presented to validate the high-order accuracy and robust performance of the hybrid scheme for steady Euler equations in curved domains with Cartesian grids.

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02014 (2/4) : 1D @E709 [Chair: Yinhua Xia]

### **[03089] Error estimates to smooth solutions of high order Runge–Kutta discontinuous Galerkin method for scalar nonlinear conservation laws with and without sonic points**

**Format :** Talk at Waseda University

**Author(s) :** Qiang Zhang (Nanjing University)

**Abstract :** In this talk we shall take the fourth order in time Runge–Kutta discontinuous Galerkin method, as an example of high order schemes, to establish a sharp a priori  $L^2$ -norm error estimates for sufficiently smooth solutions of one-dimensional scalar nonlinear conservation laws. The optimal order of accuracy in time is obtained under the standard Courant-Friedrichs-Lowy condition, and the quasi-optimal and/or optimal order of accuracy in space are achieved for many widely-used numerical fluxes, no matter whether the exact solution contains sonic points or not. Note that the convergence order in space strongly depends on the relative upwind effect of the used numerical flux, which is related to the local flowing speed and the strength of the numerical viscosity provided by the used numerical flux. Two main tools are used in this talk. One is the matrix transferring process, based on the temporal differences of stage errors. It gives a useful energy equation and help us to get the theoretical result under the acceptable temporal-spatial condition. The other is the generalized Gauss-Radau projection of the reference functions, which depends on the relative upwind effect and helps us to achieve the optimal order in space in many cases. Finally some numerical experiments are given to support the theoretical results.

### **[02994] Energy stable discontinuous Galerkin methods for compressible Navier–Stokes–Allen–Cahn System**

**Format :** Talk at Waseda University

**Author(s) :** Qiaolin He (Sichuan University)Xiaoding Shi (Beijing University of Chemical Technology)

**Abstract :** In this work, we present a fully discrete local discontinuous Galerkin (LDG) finite element method combined with scalar auxiliary variable (SAV) approach for the compressible Navier–Stokes–Allen–Cahn (NSAC) system. We start with a linear and first order scheme for time discretization and the minimal dissipation LDG for spatial discretization, which is based on the SAV approach and is proved to be unconditionally energy stable for one dimensional case. The velocity, the density and the mass concentration of fluid mixture can be solved separately. In addition, a semi-implicit spectral deferred correction (SDC) method combined with the first order scheme is employed to improve the temporal accuracy. Due to the local properties of the LDG methods, the resulting algebraic equations at the implicit level are easy to implement. In particular, we use efficient and practical multigrid solvers to solve the resulting algebraic equations. Although there is no proof of stability for the semi-implicit SDC with LDG spatial discretization, numerical experiments of the accuracy and long time simulations are presented to illustrate the high order accuracy in both time and space, the discretized energy stability, the capability and efficiency of the proposed method. Numerical results show that the initial state determines the long time behavior of the diffusive interface for the two-phase flow, which are consistent with theoretical asymptotic stability results.

### **[02714] Superconvergence of LDG method for nonlinear convection-diffusion equations**

**Format :** Talk at Waseda University

**Author(s) :** Xiong Meng (Harbin Institute of Technology)

**Abstract :** In this talk, we present superconvergence properties of the local discontinuous Galerkin (LDG) methods for solving nonlinear convection-diffusion equations in one space dimension. The main technicality is an elaborate estimate to terms involving projection errors. By introducing a new projection and constructing some correction functions, we prove the  $(2k+1)$ th order superconvergence for the cell averages and the numerical flux in the discrete  $L^2$  norm with polynomials of degree  $k \geq 1$ , no matter whether the flow direction  $f'(u)$  changes or not. Superconvergence of order  $k+2$  ( $k+1$ ) is obtained for the LDG error (its derivative) at interior right (left) Radau points, and the convergence order for the error derivative at Radau points can be improved to  $k+2$  when the direction of the flow doesn't change. Finally, a supercloseness result of order  $k+2$  towards a special Gauss-Radau projection of the exact solution is shown. The superconvergence analysis can be extended to the generalized

numerical fluxes and the mixed boundary conditions. All theoretical findings are confirmed by numerical experiments.

## [03001] An essentially oscillation-free discontinuous Galerkin method for hyperbolic conservation laws

**Format :** Talk at Waseda University

**Author(s) :** Yong Liu (ICMSEC, AMSS, CAS)Jianfang Lu (South China University of Technology)Chi-Wang Shu (Brown University)

**Abstract :** In this talk, we propose a novel discontinuous Galerkin (DG) method to control the spurious oscillations when solving the scalar hyperbolic conservation laws. The spurious oscillations may be harmful to the numerical simulation, as it not only generates some artificial structures not belonging to the problems but also causes many overshoots and undershoots that make the numerical scheme less robust. To overcome this difficulty, we introduce a numerical damping term to control spurious oscillations based on the classic DG formulation. Compared to the classic DG method, the proposed DG method still maintains many good properties, such as the extremely local data structure, conservation, L2-boundedness, optimal error estimates, and superconvergence. We also extend our methods to systems of hyperbolic conservation laws. Entropy inequalities are crucial to the well-posedness of hyperbolic conservation laws, which help to select the physically meaningful one among the infinite many weak solutions. By combining with quadrature-based entropy-stable DG methods, we also developed the entropy-stable OFDG method. For time discretizations, the modified exponential Runge--Kutta method can avoid additional restrictions of time step size due to the numerical damping. Extensive numerical experiments are shown to demonstrate our algorithm is robust and effective.

02014 (3/4) : 1E @E709 [Chair: Qi Tao]

## [03431] Structure-preserving methods for Boltzmann continuous slowing down equations

**Format :** Talk at Waseda University

**Author(s) :** Vincent Bosboom (University of Twente)Herbert Egger (Johannes Kepler Universität)Matthias Schlottbom (University of Twente)

**Abstract :** We discuss the linearized Boltzmann equation (LBE) describing the transport of particles under the influence of the Lorentz force and (inelastic) scattering. For this purpose, we consider the equation in the continuous slowing down approximation (CSDA).

We present a high-order discretization of the equation based on a mixed finite element  $P_N$  approximation that preserves the energy-conserving/dissipating nature of the different physical processes.

Additionally, we provide stability estimates of our discretization and present some numerical examples.

## [03359] Positivity-preserving high-order DG method for weakly compressible two-phase flows

**Format :** Talk at Waseda University

**Author(s) :** Fan Zhang (University of Science and Technology Beijing)

**Abstract :** This work focuses on the development of a high-order DG method for solving a three-equation model of weakly compressible two-phase flows. A novel WENO limiter and a positivity-preserving limiter are designed and applied in the numerical simulations. Moreover, we prove that the proposed method satisfies the uniform-pressure-velocity criterion which is a necessary condition for maintaining an oscillation-free phase interface.

## [03039] On Entropy Conservative and Stable Discontinuous Galerkin Spectral Element Methods

**Author(s) :** Gero Schnücke (Friedrich Schiller University Jena)

**Abstract :** The construction of high order numerical methods to solve conservation laws and related equations includes the

approximation of non-linear flux terms in the volume integrals. This terms can lead to aliasing and stability issues, e.g. due to under-resolution of vortical structures. The nodal discontinuous Galerkin spectral element method (DGSEM)

contains that discrete derivative approximations in space are summation-by-parts (SBP) operators. Furthermore, in order to avoid aliasing errors by the interpolation operator in the volume integrals, the split form DG framework from

Gassner et al. (1) is used in these methods. The SBP property and suitable two-point flux functions in the split form DG framework allow to mimic results from the continuous entropy analysis on the discrete level. In particular, semi-discrete DGSEM can be constructed as provable entropy conservative or entropy dissipative schemes.

Numerical experiments as well as results from the simulation of turbulent flows around airfoils will be presented to validate the capabilities of these methods.

(1) Gassner G. J., Winters A. R. and Kopriva D. A. Split form nodal discontinuous Galerkin schemes with summation-by-parts property for the compressible Euler equations. *Journal of Computational Physics* 327 (2016): 39-66.

(2) Krais, N., Schnücke, G., Boilemann, T. and Gassner G. J. Split form ALE discontinuous Galerkin methods with applications to under-resolved turbulent low-Mach number flows. *Journal of Computational Physics* 421 (2020): 109726.

## [03065] Affine-Invariant WENO Weights and their applications for hyperbolic conservation laws

**Author(s)** : Wai Sun Don (Ocean University of China)

**Abstract** : Novel weights are devised for the Ai-WENO operator to reconstruct a function that undergoes an affine transformation. The WENO reconstruction and affine transformation become commutable for any given sensitivity parameter, as proven theoretically and validated numerically. The Ai-WENO scheme satisfies the ENO property and is intrinsically well-balanced. Examples in the shallow water wave equations and the Euler equations under gravitational fields are given. An Ai-WENO scheme enhances robustness and reliability for solving hyperbolic conservation laws.

02014 (4/4) : 2C @E709 [Chair: Yong Liu]

## [03094] Arbitrary high-order fully-decoupled numerical schemes for phase-field models of two-phase incompressible flows

**Format** : Talk at Waseda University

**Author(s)** : Ruihan Guo (Zhengzhou University)

**Abstract** : Due to the coupling between the hydrodynamic equation and the phase-field equation in two-phase incompressible flows, it is desirable to develop efficient and high-order accurate numerical schemes that can decouple these two equations. One popular and efficient strategy is adding an explicit stabilizing term to the convective velocity in the phase-field equation to decouple them. The resulting numerical methods are only first-order accurate in time, and it seems extremely difficult to generalize the idea of stabilization to the second-order version or higher. In this talk, we employ the spectral deferred correction method to improve the temporal accuracy, based on the first-order decoupled and energy stable scheme constructed by the stabilization idea. The novelty lies in how decoupling and linear implicit properties are maintained to improve efficiency. Within the framework of the spatially discretized local discontinuous Galerkin method, the resulting numerical schemes are fully decoupled, efficient, and high-order accurate in both time and space. Numerical experiments are performed to validate the high order accuracy and efficiency of the methods for solving phase-field models of two-phase incompressible flows.

## [03096] Accuracy-enhancement of discontinuous Galerkin methods for PDEs containing high-order spatial derivatives

**Format** : Talk at Waseda University

**Author(s)** : Qi Tao (Beijing University of Technology)Liangyue Ji (Milton Keynes College)Jennifer K. Ryan (KTH Royal Institute of Technology in Stockholm)Yan Xu (University of Science and Technology of China)

**Abstract** : In this talk, we shall first introduce the accuracy-enhancement of discontinuous Galerkin (DG) methods for solving PDEs with high-order spatial derivatives. It is well known that there are highly oscillatory errors for finite element approximations to PDEs that contain hidden superconvergence points. To exploit this information, a Smoothness-Increasing Accuracy Conserving (SIAC) filter is used to create a superconvergence filtered solution. This is accomplished by convolving the DG approximation against a B-spline kernel. We then present theoretical error estimates in the negative-order norm for the local DG (LDG) and ultra-weak local DG (UWLDG) approximations to PDEs containing high order spatial derivatives. Numerical results will be shown to confirm the theoretical results.

## [03105] A discontinuous Galerkin method for the Camassa-Holm-Kadomtsev-Petviashvili type equations

**Format :** Talk at Waseda University

**Author(s) :** Qian Zhang (Harbin Institute of Technology, Shenzhen )Yan Xu (University of Science and Technology of China)Yue Liu (The University of Texas at Arlington)

**Abstract :** This paper develops a high-order discontinuous Galerkin (DG) method for the Camassa-Holm-Kadomtsev-Petviashvili (CH-KP) type equations on Cartesian meshes. The significant part of the simulation for the CH-KP type equations lies in the treatment for the integration operator  $\partial^{-1}$ . Our proposed DG method deals with it element by element, which is efficient and applicable for most solutions. Using the instinctive energy of the original PDE as a guiding principle, the DG scheme can be proved as an energy stable numerical scheme. In addition, the semi-discrete error estimates results for the nonlinear case are derived without any priori assumption. Several numerical experiments demonstrate the capability of our schemes for various types of solutions.

## [03349] High order finite difference WENO methods with unequal-sized sub-stencils for the DP type equations

**Author(s) :** Xinghui Zhong (Zhejiang University)

**Abstract :** In this talk, we present finite difference weighted essentially non-oscillatory (WENO) schemes with unequal-sized sub-stencils for solving the Degasperis-Procesi (DP) and  $\mu$ - Degasperis-Procesi ( $\mu$ DP) equations, which contain nonlinear high order derivatives, and possibly peakon solutions or shock waves. By introducing auxiliary variable(s), we rewrite the DP equation as a hyperbolic-elliptic system, and the  $\mu$ DP equation as a first order system. Then we choose a linear finite difference scheme with suitable order of accuracy for the auxiliary variable(s), and finite difference WENO schemes with unequal-sized sub-stencils for the primal variable. Comparing with the classical WENO scheme which uses several small stencils of the same size to make up a big stencil, WENO schemes with unequal-sized sub-stencils are simple in the choice of the stencil and enjoy the freedom of arbitrary positive linear weights. Another advantage is that the final reconstructed polynomial on the target cell is a polynomial of the same degree as the polynomial over the big stencil, while the classical finite difference WENO reconstruction can only be obtained for specific points inside the target interval. Numerical tests are provided to demonstrate the high order accuracy and non-oscillatory properties of the proposed schemes.

# [02015] Theory and applications of random/non-autonomous dynamical systems part II

**Session Time & Room :** 1D (Aug.21, 15:30-17:10) @F309

**Type :** Proposal of Minisymposium

**Abstract :** Dynamical systems evolving in the existence of noise, is called random dynamical systems. The basic properties, such as stability, bifurcation, and statistical properties, of such random or non-autonomous dynamical systems have not been well studied in mathematics and physics. Recently, cooperative research on random dynamical systems has been developed in the fields in statistical and nonlinear physics, dynamical system theory, ergodic theory, and stochastic process theory. In this mini-symposium, we consider theory and applications of random dynamical systems. In Part II, we discuss Newton methods and random dynamical systems.

**Organizer(s) :** Hiroki Sumi, Yuzuru Sato, Kouji Yano, Takuma Akimoto

**Classification :** 37H05, 90C52, 30D05, 65K10, 37F10

**Minisymposium Program :**

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02015 (1/1) : 1D @F309 [Chair: Hiroki SUMI and Mark COMERFORD]

## [03870] Worked out examples of Random Relaxed Newton's Methods

**Format :** Talk at Waseda University

**Author(s) :** Takayuki Watanabe (Chubu University)

**Abstract :** We give some numerical results on Random Relaxed Newton's Methods which were proposed by Sumi to compute an approximate root of a given polynomial. He proved that this randomized algorithm almost surely

works well if large noise is inserted. In this talk, we demonstrate by numerical experiments that even small noise can make the randomized algorithm successful, and discuss a mathematical conjecture.

## [02705] Complex two-dimensional random relaxed Newton's methods

**Format :** Talk at Waseda University

**Author(s) :** Hiroki Sumi (Kyoto University)

**Abstract :** We develop the theory of random dynamical systems of meromorphic maps on the complex two-dimensional projective space and we consider complex two-dimensional random relaxed Newton's methods to find backward images of the origin (0,0) in  $C^2$  under complex two dimensional regular polynomial maps on  $C^2$ . We will see the randomness or noise in the systems bring us very nice things, noise-induced order and collapsing of nasty attractors, which cannot hold in deterministic relaxed Newton's methods.

## [02999] New Q-Newton's method and Backtracking line search

**Format :** Talk at Waseda University

**Author(s) :** Tuyen Trung Truong (University of Oslo)

**Abstract :** New Q-Newton's method is a variant of Newton's method which preserves the fast rate of convergence while having the additional good property of being able to avoid saddle points. It works by adding a term into the Hessian, and change the sign of negative eigenvalues. Backtracking line search boosts the convergence guarantee. This talk will describe the algorithm, good experimental performance (including finding roots of meromorphic functions), and good theoretical guarantees.

## [05306] A Universal Fatou Component

**Format :** Talk at Waseda University

**Author(s) :** Mark David Comerford (University of Rhode Island)

**Abstract :** We show that, for the non-autonomous iteration of polynomials with suitably bounded degrees and coefficients, it is possible to obtain the whole of the classical schlicht family of normalized univalent functions on the unit disc as limit functions on a single Fatou component for a single bounded sequence of quadratic polynomials.

# [02017] Recent progress in theory and applications of time-delay systems

**Session Time & Room :**

02017 (1/3) : 5B (Aug.25, 10:40-12:20) @G402

02017 (2/3) : 5C (Aug.25, 13:20-15:00) @G402

02017 (3/3) : 5D (Aug.25, 15:30-17:10) @G402

**Type :** Proposal of Minisymposium

**Abstract :** Time delays appear in several disciplines from engineering and natural sciences. Theory of delay differential equations and infinite dimensional dynamical systems has been extensively developed. Together with the development, applications of time-delay systems have been conducted in several fields including mechanistic engineering and biological sciences. In this mini-symposium, presenting recent progress in the research of time-delay systems from theoretical and application points of view, we aim to promote discussion and collaboration on theoretical and applied research and even deepen our understanding towards the time-delay systems and extend the spectrum of the applications.

**Organizer(s) :** Kota Ikeda, Tetsuya Ishiwata, Yukihiko Nakata, Junya Nishiguchi

**Classification :** 34K05, 34K60, 93C43

**Minisymposium Program :**

02017 (1/3) : 5B @G402 [Chair: Kota Ikeda]

## [04818] Delay induced self-sustained oscillations in the Nonlinear Noisy Leaky Integrate and Fire model for networks of neurons.

**Format :** Talk at Waseda University

**Author(s) :** Pierre Roux (Mathematical Institute, University of Oxford)

**Abstract :** The emergence of patterned activity in a neural networks is a key process in human and animal brains. However, since they often arise from the interplay between a large number of cells, these mechanisms are very difficult to encompass without the use of simple, consistent and self-contained mathematical models. In this talk, I will present a time-delayed nonlinear partial differential equation, the so-called Nonlinear Noisy Leaky Integrate and Fire (NNLIF) model. In a recent work, my collaborators Kota Ikeda, Delphine Salort, Didier Smets and myself have obtained some new results and insights about the emergence and the shape of periodic self-sustained oscillations in this model. In particular, we have found and studied a simplified version of the problem in the form of a delayed differential equation.

## [04601] Global stability of multi-cell reaction systems with arbitrary time delays

**Format :** Talk at Waseda University

**Author(s) :** Hirokazu Komatsu (National Institute of Technology Toyota College)

**Abstract :** In the present talk, we consider the stability of multi-cell chemical reaction systems with arbitrary time delays for each reaction, in which each intracellular chemical reaction network is weakly reversible and has zero deficiency. By constructing a Lyapunov functional and assuming additional conditions, we can show that any positive solution to the delay differential equation for the system with mass action kinetics globally converges to a positive equilibrium point in the functional state space.

## [04324] Time lag monotonicity-breaking in time-delay systems with impulses

**Format :** Talk at Waseda University

**Author(s) :** Kevin Church (CIBC)

**Abstract :** In this talk, we prove that the solution manifold concept for differential equations with state-dependent delay (DE-SDD) has no "topologically generic" analogue for DE-SDD with impulses. Precisely, the existence of a semiflow is conditional on monotonicity of the time lag. We demonstrate pathologies that occur in the monotonicity-breaking case, which in some instances lead to dynamical behaviour completely different from what is possible in DE-SDD or impulsive differential equations with constant delays.

## [03244] Mode Selection Rules for multi-Delay Systems

**Format :** Talk at Waseda University

**Author(s) :** Kin'ya Takahashi (Kyushu Institute of Technology)Taizo Kobayashi (Kyushu University )

**Abstract :** We investigate mode selection rules at the first bifurcation for a two-delay system. Selected modes are sensitively changed with the ratio of two delay times, but obey a definite selection rule if the strengths of two delays are fixed. When the strength of the short delay takes negative values, different types of mode selection rules are observed. We explore the underlying mechanism of the change of mode selection rules in the singular perturbation limit.

02017 (2/3) : 5C @G402 [Chair: Junya Nishiguchi]

## [04187] Blow-up of solutions to some delay differential equations

**Format :** Talk at Waseda University

**Author(s) :** Tetsuya Ishiwata (Shibaura Institute of Technology)Yukihiko Nakata (Aoyama Gakuin University)

**Abstract :** Time lags sometimes play an essential role in the phenomena, and it is also well-known that the delay effects cause instability or oscillation.

In this talk, we consider the effects of time delay for such instabilities from the viewpoint of a finite time blow-up of the solutions and treat some delay differential equations.

We show mathematical results on the blow-up of solutions and give numerical observations.

## [03602] Absolute stability and absolute hyperbolicity in systems with time-delays

**Format :** Online Talk on Zoom

**Author(s) :** Serhiy Yanchuk (Potsdam Institute for Climate Impact Research)

**Abstract :** We present criteria for the absolute stability of DDEs. For a single delay, the absolute stability is shown to be equivalent to asymptotic stability for sufficiently large delays. For multiple delays, the absolute stability is equivalent to asymptotic stability for hierarchically large delays. Additionally, we give necessary and sufficient conditions for a linear DDE to be hyperbolic for all delays. The latter conditions are crucial for determining whether a system can have bifurcations.

## [03557] Delay-dependent stability switches in delay differential systems

**Format :** Talk at Waseda University

**Author(s) :** Hideaki Matsunaga (Osaka Metropolitan University)

**Abstract :** We will summarize some recent results on the stability properties of linear differential systems with delays. Some examples are provided to illustrate the delay-dependent stability switches for a system with delay in the diagonal terms. The proof technique is based on careful analysis of the existence and the transversality of characteristic roots on the imaginary axis. This is a joint work with Yuki Hata.

## [05023] Stabilization of periodic orbits with complex characteristic multipliers via DFC

**Format :** Talk at Waseda University

**Author(s) :** Rinko Miyazaki (Shizuoka Univ.)Dohan Kim (Seoul National University)Jong Son Shin (Shizuoka University)

**Abstract :** The delayed feedback control (DFC) proposed by Pyragas (Pyhs. Lett. A, 1992) is a method to stabilize an unstable periodic orbit by using delayed terms. Recently we have succeeded in proving a stabilization regime under certain constraints. In this talk, we will focus on the case where the characteristic multiplier is complex.

02017 (3/3) : 5D @G402 [Chair: Yukihiko Nakata]

## [03942] “Mild solutions” for hereditary linear differential systems

**Format :** Talk at Waseda University

**Author(s) :** Junya Nishiguchi (Tohoku University)

**Abstract :** In this talk, we discuss the variation of constants formula for delay differential equations by introducing the notion of a mild solution, which is a solution under an initial condition having a discontinuous history function. Then the principal fundamental matrix solution is defined as a matrix-valued mild solution, and we obtain the variation of constants formula with this function.

## [04145] Linearized instability for neutral functional differential equations with state-dependent delays

**Format :** Talk at Waseda University

**Author(s) :** Jaqueline Godoy Mesquita (Universidade de Brasília)Bernhard Lani-Wayda (Justus-Liebig University)

**Abstract :** In this talk, I will present a linearized instability principle for neutral functional differential equations with state-dependent delays. Also, I will discuss open and developing problems in this field. This is a joint work with Professor Bernhard Lani-Wayda from Justus-Liebig University, in Giessen, Germany.

## [03765] Morse decomposition of the global attractor for delay differential equations

**Format :** Talk at Waseda University

**Author(s) :** Abel Garab (University of Szeged)

**Abstract :** We consider unidirectional cyclic systems of delay differential equations of the form

\begin{equation} \dot{x}^i(t) = g^i(x^i(t), x^{i+1}(t-\tau^i)), \quad 0 \leq i \leq N, \\ \end{equation}

where the indices are understood modulo  $N + 1$ . We show that if the global attractor exists, then it does not

part\_2

contain any superexponential solution (i.e. that converges to 0 faster than any exponential function). This allows us to construct a Morse decomposition of the global attractor of such equations, which is based on an integer valued Lyapunov function.

# [02023] Theory and applications of random/no-autonomous dynamical systems part IV

**Session Time & Room :** 2C (Aug.22, 13:20-15:00) @F309

**Type :** Proposal of Minisymposium

**Abstract :** Dynamical systems evolving in the existence of noise, is called random dynamical systems. The basic properties, such as stability, bifurcation, and statistical properties, of such random or non-autonomous dynamical systems have not been well studied in mathematics and physics. Recently, cooperative research on random dynamical systems has been developed in the fields in statistical and nonlinear physics, dynamical system theory, ergodic theory, and stochastic process theory. In this mini-symposium, we consider theory and applications of random dynamical systems. In Part IV, we discuss anomalous statistics and non-stationarity in random dynamical systems.

**Organizer(s) :** Hiroki Sumi, Yuzuru Sato, Kouji Yano, Takuma Akimoto

**Classification :** 37H05

**Minisymposium Program :**

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02023 (1/1) : 2C @F309 [Chair: Yuzuru sato]

## [05589] Physical applications of infinite ergodic theory

**Format :** Talk at Waseda University

**Author(s) :** Eli Barkai (Bar Ilan University)

**Abstract :** We show how non-normalised Boltzmann Gibbs measure can still yield statistical averages and thermodynamic properties of physical observables, exploiting a model of Langevin dynamics of a single Brownian particle in an asymptotically flat potential. Similar tools are applicable for a gas of sub-recoiled laser cooled atoms and weakly chaotic non-linear oscillators.

## [03122] Transition to Anomalous Dynamics in A Simple Random Map

**Format :** Talk at Waseda University

**Author(s) :** Jin Yan (Max Planck Institute for the Physics of Complex Systems)Moitrish Majumdar (International Centre for Theoretical Sciences - TIFR)Stefano Ruffo (SISSA Trieste)Yuzuru Sato (Hokkaido University)Christian Beck (Queen Mary University of London)Rainer Klages (Queen Mary University of London)

**Abstract :** A random dynamical system consists of a setting where different types of dynamics are sampled randomly in time. Here we consider a simple yet universal example, where an expanding or a contracting map is randomly selected at each discrete-time with probability  $p$  or  $1-p$ , respectively. By continuously varying  $p$  between zero and one, we found anomalous behaviour characterised by an infinite non-normalisable invariant density, weak ergodicity breaking, and a power-law decay in correlations.

## [05573] Arcsine law for random dynamics with a core

**Format :** Talk at Waseda University

**Author(s) :** Yushi Nakano (Tokai University)Fumihiro Nakamura (Kitami Institute of Technology)Hisayoshi Toyokawa (Kitami Institute of Technology)Kouji Yano (Osaka University)

**Abstract :** The arcsine law is a characterization of intermittent dynamics in infinite ergodic theory. A well-known model of intermittent dynamics is an interval with two increasing surjective branches being uniformly expanding except for indifferent fixed points at the boundary. We show that the arcsine law holds for random dynamics with a core, which is a class of random iterations of two interval maps without indifferent periodic points but "indifferent in average" at the boundary.

## [05570] Infinite ergodic theory in physics

**Format :** Talk at Waseda University

**Author(s) :** Takuma Akimoto (Tokyo University of Science)

**Abstract :** Infinite ergodic theory provides a distributional behavior of time-averaged observables in dynamical systems. We show that the infinite ergodic theory plays an important role in physics. In particular, we show several distributional limit theorems for time-averaged observables in non-stationary stochastic processes that are models of anomalous diffusion and laser-cooled systems.

## [02025] Recent Advances on the Analysis and Applications of Continuous and Discrete Integrable Systems

**Session Time & Room :**

02025 (1/3) : 3C (Aug.23, 13:20-15:00) @F310

02025 (2/3) : 3D (Aug.23, 15:30-17:10) @F310

02025 (3/3) : 3E (Aug.23, 17:40-19:20) @F310

**Type :** Proposal of Minisymposium

**Abstract :** Research in integrable systems has led to numerous important new concepts, ideas and techniques of mathematics and physics in the last few decades. The very concept of integrability has been found in deep connections with a large spectrum of mathematics such as algebraic geometry, differential geometry, representation theory, random matrix theory, nonlinear waves, etc. In this minisymposium, we will focus on the recent developments of both continuous and discrete integrable systems. Specially, it will cover discrete and ultradiscrete integrable systems, noncommutative integrable systems and rogue waves. This is a unique platform for the interaction of international researchers in relevant fields.

**Organizer(s) :** Kenichi Maruno, Linyu Peng, Cheng Zhang

**Classification :** 39A36, 37K10, 35Q51, 37J70, 35C08

**Minisymposium Program :**

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02025 (1/3) : 3C @F310 [Chair: Linyu Peng]

## [03558] Integrable boundary conditions for quad-graph systems: classification and applications

**Format :** Talk at Waseda University

**Author(s) :** Cheng Zhang (Shanghai University)

**Abstract :** The notion of boundary conditions for quad-graph systems will first be introduced. The boundary conditions are naturally defined on triangles that arise as dualization of given quad-graphs with boundary. For three-dimensionally consistent quad-graph systems, the so-called integrable boundary conditions will be characterized as boundary conditions satisfying the boundary consistency condition that is a consistency condition defined on a half of a rhombic-dodecahedron. Based on these notions, three main results will then be presented: a classification of integrable boundary conditions for quad-equations of the ABS classification; Lax formulations of integrable boundary conditions; and the so-called open boundary reduction technique as systematic a means to construct integrable mappings from integrable initial-boundary value problems for quad-graph systems.

## [03221] Geometric Aspects of Miura Transformations

**Format :** Talk at Waseda University

**Author(s) :** Changzheng Qu (Ningbo University) Zhiwei Wu (Sun Yat-sen University)

**Abstract :** The Miura transformation and its extensions play a crucial role in the study of integrable systems, which have been used to relate different kinds of integrable equations and to classify the bi-Hamiltonian structures. In this talk, we will discuss the geometric aspects of the Miura transformation. The generalized Miura transformations from the mKdV-type hierarchies to the KdV-type hierarchies are constructed under both algebraic and geometric settings. We show that the Miura transformations not only relate integrable curve flows in different part\_2

geometries but also induce the transition between different moving frames. Moreover, the Miura transformation gives the factorization of generating operators of constraint Gelfand-Dickey hierarchy. This talk is based on a recent joint work with Prof. Qu, Changzheng.

### [04193] Curvature equation with conic singularities and integrable system

**Format :** Talk at Waseda University

**Author(s) :** Ting-Jung Kuo (National Taiwan Normal University)

**Abstract :** Let  $(E_\tau, dz^2)$ ,  $\tau \in \mathbb{H}$  be a flat torus. We consider the following PDE:

\begin{equation}

$\Delta u + e^u = \sum_{j=1}^N p_j \alpha_j \delta_{p_j} \text{ on } E$

E\tau -(1)

\end{equation}

where  $\delta_{p_j}$  is the dirac measure and  $\alpha_j$  for  $j > -1$

. In the literature, equation (1) arises from conformal geometry. Indeed, (1) is equivalent to saying that the conformal metric  $ds^2 = \frac{1}{2} e^{2u} dz \wedge d\bar{z}$

with conic singularities at  $p_j$  has the Gaussian curvature 1. By classical Liouville theorem, the curvature equation is also an integrable system which yields a complex ODE (a generalization of the classical Lame equation) and the solvability of equation (1) is equivalent to saying that the corresponding complex ODE is always apparent and has unitary monodromy. The study of the monodromy of a general complex ODE is difficult in general. However, recently, we also discover its relation with KdV theory. In this talk, I will talk about this deep connection and focus on the study of the complex ODE from monodromy point of view.

### [03194] A Generalization of an Integrability Theorem of Darboux and the Stable Configuration Condition.

**Format :** Talk at Waseda University

**Author(s) :** Irina A. Kogan (North Carolina State University)

**Abstract :** In his monograph "Systemes Orthogonaux" (1910), Darboux stated three theorems providing local existence and uniqueness of solutions to first order systems of PDEs, where for each unknown function a certain subset of partial derivatives is prescribed and the values of the unknown functions are prescribed along transversal coordinate affine subspaces. The more general of the theorems, Theorem III, was proved by Darboux only for the cases of 2 and 3 independent variables. We formulate and prove a generalization of Theorem III. Instead of partial derivatives, we prescribe derivatives of the unknown functions along vector fields. The values of the unknown functions are prescribed along arbitrary transversal submanifolds. We identify a certain Stable Configuration Condition (SCC). This is a geometric condition that depends on both the set of vector fields and on the initial manifolds. SCC is automatically met in the case considered by Darboux. Assuming the SCC and the relevant integrability conditions are satisfied, we establish local existence and uniqueness of a  $C^1$ -smooth solution via Picard iteration for any number of independent variables. If the SCC is not satisfied, we show on a concrete example that the uniqueness can fail the following strong sense: for the same initial data, there are two solutions that differ on any open subset of their domains. This talk is based on joint publications with Michael Benfield and Kris Jenssen.

02025 (2/3) : 3D @F310 [Chair: Cheng Zhang]

### [03560] Rogue waves and their patterns in the vector nonlinear Schrödinger equation

**Format :** Talk at Waseda University

**Author(s) :** Baofeng Feng (University of Texas Rio Grande Valley) Peng Huang (Shenzhen University) Chengfa Wu (Shenzhen University) Guangxiong Zhang (Shenzhen University)

**Abstract :** This talk presents the general rogue wave solutions and their patterns in the vector (or M-component) nonlinear Schrödinger (NLS) equation. We derived the explicit solution for the rogue wave expressed by tau-functions that are determinants of  $K \times K$  block matrices with an index jump of  $M+1$ . Patterns of the rogue waves for  $M=3,4$  and  $K=1$  are thoroughly investigated.

## [03656] Whitham modulation theory of Riemann problem for nonlinear integrable equations

**Format :** Talk at Waseda University

**Author(s) :** Yaqing Liu (Beijing Information Science and Technology University)

**Abstract :** The Riemann problem of the nonlinear integrable equation with step-like initial value is explored by Whitham modulation theory, which is a modified version of the well-known finite-gap integration method. Based on the reparameterization of the solution with the use of algebraic resolvent of the polynomial defining the solution, the periodic wave solutions of the nonlinear integrable equation are described by the elliptic function along with the Whitham modulation equations. Complete classification of possible wave structures is given for all possible jump conditions at the discontinuity initial value. The proposed analytic results are confirmed through direct numerical simulations.

## [03369] Quantum variational principle for Lagrangian 1-forms

**Format :** Talk at Waseda University

**Author(s) :** Sikarin Yoo-Kong (Naresuan University)

**Abstract :** In this talk, we will present a new type of the propagator associated with the Lagrangian 1-forms called the (continuous) multi-time propagator. With this new type of the propagator, a new paradigm on summing over possible paths arises since one needs to take into account not only summing over possible spatial paths but also summing over possible temporal paths. The quantum intragrability (a.k.a multi-dimensional consistency), which mainly relies on the classical Lagrangian 1-form closure relation, will be captured in the language of Feynman path integration.

## [05098] Three-dimensional fundamental diagram of stochastic cellular automata

**Format :** Talk at Waseda University

**Author(s) :** Kazushige Endo (Kindai University)

**Abstract :** Cellular automata including Burgers cellular automaton are not only examples of ultradiscrete analogue of integrable systems, but also mathematical models which show fundamental mechanisms of traffic flow. For example, a phase transition from free flow to congested flow in a traffic system is well-known and has been studied using fundamental diagram. Fundamental diagram is an object showing relation between the density of traffic (particles) and their mean momentum. However, the density of particles is not a unique parameter to determine the mean momentum. Several systems whose mean momentum is uniquely determined by a pair of the density and another conserved quantity have been discovered. In this talk, we show a three-dimensional framework of the fundamental diagram of stochastic cellular automata and its theoretical derivation.

02025 (3/3) : 3E @F310 [Chair: Kenichi Maruno]

## [05088] Beyond the Painlevé property

**Format :** Talk at Waseda University

**Author(s) :** Rod Halburd (University College London)

**Abstract :** The Painlevé property and associated tests have led to the identification of integrable cases of many families of equations. In this talk I will describe some generalisations of the Painlevé property that allow for the identification of a wider set of integrable equations. Various necessary conditions will be discussed and implemented. Examples from Newtonian and relativistic stellar models will be analysed

## [05195] Constructing non-commutative systems with Pfaffian type solutions

**Format :** Talk at Waseda University

**Author(s) :** Claire Gilson (University of Glasgow)

**Abstract :** In this talk we look to construct non-commutative systems from quasi-determinants of Pfaffian type by considering quasi-determinant identities.

## [03957] Addition formulae for ultradiscrete hafnians

**Format :** Talk at Waseda University

**Author(s) :** Hidetomo Nagai (Tokai University)

**Abstract :** Ultradiscrete hafnian is an ultradiscrete analogue of hafnian, which is signature free pfaffian. In this talk we propose some formulae for the ultradiscrete hafnians with some conditions, which are related to the ultradiscrete soliton solutions.

## [05092] Recent Advances on the Analysis and Applications of Continuous and Discrete Integrable Systems

**Format :** Talk at Waseda University

**Author(s) :** Andrew Hone (University of Kent)

**Abstract :** "New discrete integrable systems from deformed cluster mutations"

We describe how to obtain integrable maps by deforming cluster algebra mutations that display Zamolodchikov periodicity. The simplest example is the general Lyness map in 2D, arising as a 2-parameter family of deformations of the cluster algebra of finite type A\_2. Results will be presented on integrability of deformed mutations in type A\_n, and other finite root systems. This is joint work with J.Grabowski, W.Kim, and T.Kouloukas.

## [02056] Recent Advances in Partitioning Method for the Structures

**Session Time & Room :**

02056 (1/2) : 2D (Aug.22, 15:30-17:10) @E802

02056 (2/2) : 2E (Aug.22, 17:40-19:20) @E802

**Type :** Proposal of Minisymposium

**Abstract :** Despite numerous well-established algebraic techniques, infusion of the variational approach into computational mechanics is still under way. Among those, the partitioning method has played a pivotal role. It introduced a complicated matrix computation and additional unknowns which should be treated without degrading accuracy. Topics of this mini-symposium will include, but not limited to, the advances in partitioning method and their application; parallel computing, component mode synthesis, non-matching interface, inverse problems, and damage detection. The mini-symposium will bring researchers together working on both fundamental and applied aspects of computational mechanics to provide a forum for discussion, interaction, and assessment of techniques.

**Organizer(s) :** SangJoon Shin

**Classification :** 65Nxx, 74Sxx, 65Fxx, 65Yxx, 74Hxx

**Minisymposium Program :**

02056 (1/2) : 2D @E802 [Chair: SangJoon Shin]

## [03920] Displacement-only Partitioned Equations for Structures without Lagrange Multipliers

**Format :** Talk at Waseda University

**Author(s) :** K. C. Park (University of Colorado)

**Abstract :** A new formulation for the Displacement-only Partitioned (DP) equations of motion for linear structures is presented,

which employs: the partitioned displacement and applied force ( $u, f$ ), the partitioned block diagonal mass and stiffness matrices ( $M, K$ ); and, the coupling projector ( $P$ ), yielding the partitioned coupled equations of motion:

$$M \ddot{u} = P(f - Ku)$$

The proposed DP formulation contains no Lagrange multipliers and offers wide practical applications as well as intellectual pleasure.

## [04749] Displacement-based dynamic analysis of partitioned structural systems

**Format :** Online Talk on Zoom

**Author(s) :** José Ángel González Pérez (Universidad de Sevilla)K. C. Park (University of Colorado)

**Abstract :** An unconditionally stable implicit-explicit time integration algorithm is presented, which employs the displacement-only partitioned formulation for structures. The displacement-only partitioned equations of motion for linear and nonlinear structures are expressed in terms of the partitioned displacements, partitioned velocities, and partitioned accelerations, and are devoid of interface Lagrange multipliers and associated variables. Numerical examples illustrate both unconditional stability of the proposed algorithm, second-order accuracy, as well as computational simplicity and efficiency.

## [04659] Partitioned Damage Identification of Structural Systems

**Format :** Talk at Waseda University

**Author(s) :** Hyeon-Jun Kim (KAIST)Yong-Hwa Park (KAIST)K. C. Park (University of Colorado)

**Abstract :** This study proposes a damage identification procedure by employing a recently developed displacement-only partitioned equations of motion for structures. Damage is identified by detecting changes in partitioned or elemental stiffness. Applications of the proposed damage identification procedure to sample problems show that the proposed procedure captures damage locations through numerical examples.

02056 (2/2) : 2E @E802 [Chair: K. C. Park]

## [03098] Development of partitioning method for thermoelastic Interaction Problems with energy flux constraint

**Format :** Online Talk on Zoom

**Author(s) :** Chang-uk Ahn (Kyung Hee University)Alexandre Cortiella (University of Colorado)Jin-gyun Kim (Kyung Hee University)Kwang-chun park (Korea Advanced Institute of Science and Technology)

**Abstract :** This study presents a partitioned symmetric formulation for transient thermoelastic interaction problems. The thermoelastic interaction problem is a multiphysics problem in which the wave (i.e., hyperbolic type) equation and the diffusion (i.e., parabolic type) equation are coupled. The classical formulation of thermoelastic problems is non-symmetric, and its partitioned form has only been developed in ways that the domains are decoupled in the discrete domain. Based on this motivation, we propose a constraint of energy flux that allows partitioning the thermoelastic problem in a continuum domain. To do this, we construct two separate variational formulations of the uncoupled thermal conduction and uncoupled structural systems. In other words, two separate variational formulations of the uncoupled thermal conduction and uncoupled structural systems are augmented by the constraint of energy exchanges between the elastic body and the thermal conduction body via the method of Lagrange multipliers.

Finally, this study introduces a solution algorithm including implicit-implicit time integration strategies, and the present partitioned formula is verified by well-organized numerical examples.

## [04222] A Componenet Mode Synthesis Method Using a Displacement-Based Partitioned Approach

**Format :** Online Talk on Zoom

**Author(s) :** Muhammad Faizan Baqir (Kyung Hee University )K. C. Park (University of Colorado)Jin Gyun Kim (Kyung Hee University)

**Abstract :** A new Partitioned component mode synthesis (P-CMS) is presented, which employs a recently developed Displacement-based Partitioned (DP) formalism. The reduced system matrices are generated via block-by-block substructural matrix computations, directly yielding reduced-order models. The proposed P-CMS method can provide a robust mode selection criterion that remains a challenge in most existing CMS methods. Details of the proposed P-CMS procedure along with numerical examples will be presented in this talk.

## [03460] Iterative Algorithm for Quasistatic Structural Problems Employing Only Partitioned Displacements

**Format :** Talk at Waseda University

**Author(s) :** SANGJOON SHIN (Seoul National University) Seung-Hoon Kang (Seoul National University) Kwang-Chun Park (University of Colorado Boulder)

**Abstract :** We report some initial results from the ongoing research on partitioned parallel solution of quasistatic structural problems that employ only partitioned displacements. A notable feature of the present method is the absence of Lagrange multipliers that inevitably manifest in standard partitioned formalisms. Various preconditioning and regularizations that take advantages of the present Displacement-only Partitioned (DP) formulation will be presented and compared with FETI and its allied solution methods.

## [02060] Topics in extremal graph theory

**Session Time & Room :** 4C (Aug.24, 13:20-15:00) @G302

**Type :** Proposal of Minisymposium

**Abstract :** Extremal graph theory is a fast emerging and growing area with many exciting developments in recent years. This mini-symposium will cover topics in Turan problem, sublinear expander and sparse pseudorandom graphs.

**Organizer(s) :** Jie Han, Donglei Yang

**Classification :** 05C05, 05C48, 05C35

**Minisymposium Program :**

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02060 (1/1) : 4C @G302

## [02678] Spanning trees in sparse pseudorandom graphs

**Format :** Online Talk on Zoom

**Author(s) :** Jie Han (Beijing Institute of Technology) Donglei Yang (Shandong University)

**Abstract :** Let  $\mathcal{T}(n, \Delta)$  be the class of trees with  $n$  vertices and maximum degree at most  $\Delta$ . Confirming a conjecture of Kahn, Montgomery established for every fixed tree  $T \in \mathcal{T}(n, \Delta)$ , the smallest value of  $p$  for which  $G(n, p)$  a.a.s. contains a copy of  $T$ . There have been a wealth of results and open problems on embedding spanning trees in (pseudo)random graphs in the past few decades. In 2005, Alon, Krivelevich and Sudakov asked for determining the best possible spectral gap forcing an  $(n, d, \lambda)$ -graph to be  $\mathcal{T}(n, \Delta)$ -universal. In this talk, we introduce some recent works and open questions. Similar questions for expander graphs are also considered.

## [03075] Extremal results on 4-cycles

**Format :** Talk at Waseda University

**Author(s) :** Tianchi Yang (National University of Singapore)

**Abstract :** The study of 4-cycles has important implications for the progression of Turan type problems, particularly in their degenerate forms. In this presentation, novel upper bounds are derived for the maximum number of edges in  $n$ -vertex graphs without cycles of length four. These findings not only augment our comprehension of combinatorial structures but also disprove certain conjectures of Erdos.

## [03224] Many Hamiltonian subsets in large graphs with given density

**Format :** Talk at Waseda University

**Author(s) :** Stijn Cambie (Institute for Basic Science) Jun Gao (Institute for Basic Science) Hong Liu (Institute for Basic Science)

**Abstract :** A set of vertices in a graph is a Hamiltonian subset if it induces a subgraph containing a Hamiltonian cycle. Kim, Liu, Sharifzadeh and Staden proved that among all graphs with minimum degree  $d$ ,  $K_{d+1}$  minimises the number of Hamiltonian subsets. We prove a near optimal lower bound that takes also the order and the structure of a graph into account. For many natural graph classes, it provides a much better bound than the extremal one ( $\approx 2^{d+1}$ ). Among others, our bound implies that an  $n$ -vertex  $C_4$ -free graphs with minimum degree  $d$  contains at least  $n2^{d^2-o(1)}$  Hamiltonian subsets.

This is a joint work with Stijn Cambie and Hong Liu.

## [03146] Balanced Subdivisions in Graphs

**Format :** Talk at Waseda University

**Author(s) :** Donglei Yang (Shandong University)

**Abstract :** A balanced subdivision of a graph  $H$  is obtained from  $H$  by equally subdividing every edge. In 1984, Thomassen conjectured that for each integer  $k \geq 1$ , high average degree forces a balanced subdivision of  $K_k$ , and this was recently resolved by Liu and Montgomery. We give an optimal estimate on the average degree condition forcing every balanced  $H$ -subdivision, resolving a question of Fernández et al. Similar problems on clique immersions are also considered.

## [02067] Recent topics on generalized orthogonal polynomials and their applications

**Session Time & Room :**

02067 (1/2) : 1C (Aug.21, 13:20-15:00) @G401

02067 (2/2) : 1D (Aug.21, 15:30-17:10) @G401

**Type :** Proposal of Minisymposium

**Abstract :** Orthogonal polynomials play crucial roles in a variety of fields including integrable systems, combinatorics, quantum information and so on. Generalization of orthogonal polynomials has thus been considered from many points of view and has led to successful application to such areas. This minisymposium aims to bring together latest research results on theory and applications of generalized orthogonal polynomials and aims to promote interdisciplinary discussions.

**Organizer(s) :** Satoshi Tsujimoto, Hiroshi Miki, Luc Vinet

**Classification :** 33Cxx, 05Exx, 81Rxx

**Minisymposium Program :**

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02067 (1/2) : 1C @G401 [Chair: Satoshi Tsujimoto]

## [04542] Meta algebras, biorthogonal rational functions and the Askey scheme

**Format :** Talk at Waseda University

**Author(s) :** Satoshi Tsujimoto (Kyoto University)Luc Vinet (IVADO & CRM, Université de Montréal)Alexei Zhedanov (School of Mathematics, Renmin University)

**Abstract :** Algebras that subsume those of the Askey-Wilson type and are designated by the suffix meta are introduced to explain in a unified way the bispectral properties of the orthogonal polynomials of the Askey scheme and of biorthogonal rational functions that can be associated to the entries of that scheme. The Hahn and Racah families will be used to illustrate the framework.

## [04588] Introducing $q \rightarrow -1$ limits of biorthogonal rational functions: two instructive examples

**Format :** Talk at Waseda University

**Author(s) :** Julien Gaboriaud (Kyoto University)Satoshi Tsujimoto (Kyoto University)

**Abstract :** We recall how  $q \rightarrow -1$  limits of orthogonal polynomials have been introduced and we introduce analogous limits for biorthogonal rational functions (BRF). In order to illustrate the main properties of these  $q \rightarrow -1$  BRF, we look at two "extremal" cases: the most general one (Wilson) and one of the simplest ones (Pastor).

## [03379] CMV bispectrality of polynomials orthogonal on the unit circle

**Format :** Online Talk on Zoom

**Author(s) :** Alexei Zhedanov (School of Mathematics, Renmin University)

**Abstract :** We present new explicit results and examples concerning CMV bispectrality of the polynomials orthogonal on the unit circle.

## [04976] The Element Distinctness Problem Revisited

**Format :** Online Talk on Zoom

**Author(s) :** Hajime Tanaka (Tohoku University)

**Abstract :** The element distinctness problem is the problem of deciding whether or not a list contains identical elements. In this talk, I will revisit Ambainis' famous quantum algorithm for the problem (2007) and its refinement by Portugal (2018) in terms of the Grover quantum walk on the Johnson graphs. I will explain how a result about orthogonal polynomials (i.e., Leonard pairs) plays a role here.

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02067 (2/2) : 1D @G401 [Chair: Hiroshi Miki]

## [02693] Christoffel Transformations for (Partial-)Skew-Orthogonal Polynomials and Applications

**Format :** Talk at Waseda University

**Author(s) :** Guofu Yu (Shanghai Jiao Tong University)

**Abstract :** In this talk, we consider the Christoffel transformations for skew-orthogonal polynomials and partial-skew-orthogonal polynomials. We demonstrate that the Christoffel transformations can act as spectral problems for discrete integrable hierarchies, and therefore we derive certain integrable hierarchies from these transformations. Some reductional cases are also considered. This is a joint work with Shi-Hao Li.

## [02730] Multiple skew orthogonal polynomials and two-component Pfaff lattice

**Format :** Talk at Waseda University

**Author(s) :** Shi-Hao Li (Sichuan University)

**Abstract :** The relation between orthogonal polynomials and integrable system is a long-standing focus in mathematical physics, and sheds light in many related fields like random matrices, random walks, and so on. Skew orthogonal polynomials, which were proposed in the study of random matrices with orthogonal/symplectic symmetry, were found to be wave functions for integrable systems of DKP type. In this talk, we will generalize this frame by considering multiple skew orthogonal polynomials which involve several different weights. In particular, connections with integrable systems are also considered. Pfaffian expressions, recurrence relations and Cauchy transforms for multiple skew orthogonal polynomials will be performed to give rise to multiple-component Pfaff lattice hierarchy.

## [04996] Another Type of Forward and Backward Shift Relations for Orthogonal Polynomials in the Askey Scheme

**Format :** Talk at Waseda University

**Author(s) :** Satoru Odake (Shinshu University)

**Abstract :** The forward and backward shift relations are basic properties of the (basic) hypergeometric orthogonal polynomials in the Askey scheme (Jacobi, Askey-Wilson,  $q$ -Racah, big  $q$ -Jacobi etc.) and they are related to the factorization of the differential or difference operators. Based on other factorizations, we obtain another type of forward and backward shift relations.

# [02072] Theory and applications of random/non-autonomous dynamical systems: Part I

**Session Time & Room :** 1C (Aug.21, 13:20-15:00) @F309

**Type :** Proposal of Minisymposium

**Abstract :** Dynamical systems evolving in the existence of noise, is called random dynamical systems. The basic properties, such as stability, bifurcation, and statistical properties, of such random or non-autonomous dynamical systems have not been well studied in mathematics and physics. Recently, cooperative research on random dynamical systems has been developed in the fields in statistical and nonlinear physics, dynamical system theory, ergodic theory, and stochastic process theory. In this mini-symposium, we consider theory and applications of random dynamical systems. In Part I, we discuss computational ergodic theory and applications in random dynamical systems.

**Organizer(s) :** Hiroki Sumi, Yuzuru Sato, Kouji Yano, Takuma Akimoto

**Classification :** 37H05, 37H10, 37H20

**Minisymposium Program :**

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02072 (1/1) : 1C @F309 [Chair: Yuzuru Sato]

## [03478] New characterizations of noise-induced order

**Format :** Talk at Waseda University

**Author(s) :** Yuzuru Sato (Hokkaido University)

**Abstract :** This talk includes a brief review of phenomenologies of non-autonomous / random dynamical systems, followed by a few examples of typical noise-induced phenomena in random dynamical systems.

In particular, we present recent results on new characterizations of noise-induced order.

## [04094] Time-delayed feedback control for random dynamical systems

**Format :** Talk at Waseda University

**Author(s) :** Miki Kobayashi (Rissho University)Yuzuru Sato (Hokkaido University)

**Abstract :** We propose a framework of Pyragas control for random dynamical systems. The deterministic Pyragas control adopts delayed feedback controls to stabilize a UPO in the original deterministic strange attractor. We demonstrate a few examples including stochastic Rossler dynamics.

## [03936] Rigorous enclosure of spectra and its applications

**Format :** Talk at Waseda University

**Author(s) :** Isaia Nisoli (Universidade Federal do Rio de Janeiro)Alex Blumenthal (Georgia Tech)Toby Taylor-Crush (Loughborough University)Yuzuru Sato (Hokkaido University)

**Abstract :** In this talk I will introduce a tool developed in collaboration with Dr. A. Blumenthal and Dr. T. Taylor-Crush to rigorously enclose the finite spectrum of a Markov operator. I will then introduce some applications to the study of the phenomenology of important examples of random dynamical systems developed by Prof. Y. Sato.

## [03935] Recent developments on Lorenz-like attractors

**Format :** Talk at Waseda University

**Author(s) :** MARIA JOSE PACIFICO (Federal University of Rio de Janeiro)

**Abstract :** The Lorenz attractor has been playing a central role in the research of singular flows, i.e., flows generated by smooth vector fields with singularities. In this talk I shall survey about old and new results describing the dynamics of this kind of attractors from the topological as well as the ergodic point of view. I will end sketching the proof of my result establishing that in a C1-open and densely family of vector fields (including the classical Lorenz attractor), if the point masses at singularities are not equilibrium states, then there exists a unique equilibrium state supported on  $\Lambda$ . In particular, there exists a unique measure of maximal entropy for the flow  $X|\Lambda$ .

# [02083] Integrable Aspects of Nonlinear Wave Equations, Solutions and Asymptotics

## **Session Time & Room :**

02083 (1/3) : 4C (Aug.24, 13:20-15:00) @F309

02083 (2/3) : 4D (Aug.24, 15:30-17:10) @F309

02083 (3/3) : 4E (Aug.24, 17:40-19:20) @F309

## **Type :** Proposal of Minisymposium

**Abstract :** The study of physical phenomena by means of mathematical models often leads to integrable systems, which admit rich solutions including the solitons. The study on interactions of solitary waves is an important part of the modern theory of nonlinear waves. Various methods have been developed to build their solutions. In addition, stability and long-time asymptotics of solutions to integrable systems are interesting topics and attracts much attentions in the past years.

The proposed minisymposium aims at bringing together the researchers in the fields and at offering an overview of some of the current research activities in this area.

**Organizer(s) :** Alejandro Aceves, Xingbiao Hu, Qingping Liu, Changzheng Qu

**Classification :** 37K15, 37K25, 35Q51, 37K40, 35C08

## **Minisymposium Program :**

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02083 (1/3) : 4C @F309

## **[05581] Recent results on the Fractional Nonlinear Schrödinger Equation**

**Format :** Talk at Waseda University

**Author(s) :** Alejandro Aceves (Southern Methodist University)

**Abstract :** The Fractional Nonlinear Schrödinger Equation (fNLSE) has been a topic of recent interest as it may have applications to nonnonlinear photonics. In this work we will present motivation for the models considered and recent results on discrete and continuous fNLSE.

In particular we will discuss the existence of discrete localized modes and their properties. Rigorous and numerical results on existence for the continuous fNLSE will also be presented.

## **[05588] Duality of positive and negative integrable hierarchies via relativistically invariant fields**

**Format :** Online Talk on Zoom

**Author(s) :** Senyue Lou (Ningbo University)Xing-Biao Hu (Academy of Mathematics and Systems Science, Chinese Academy of Sciences)Qingping Liu (China University of Mining and Technology (Beijing))

**Abstract :** This talk concerns the relativistic invariance in integrable systems. Using the invariant sine-Gordon, Tzitzeica, Toda fields and second heavenly equations as dual relations, some well-known continuous and discrete integrable positive hierarchies are converted to the negative hierarchies. In (1+1)-dimensional cases the positive/negative hierarchy dualities are guaranteed by the mastersymmetry method and the relativistic invariance of the duality relations. Two elegant commuting recursion operators of the heavenly equation appear naturally from the formal series symmetry approach.

## **[04900] Integrable Deep Learning--PINN based on Miura transformations and discovery of new localized wave solutions**

**Format :** Talk at Waseda University

**Author(s) :** Yong Chen (East China Normal University)

**Abstract :** We put forth two physics-informed neural network (PINN) schemes based on Miura transformations. The novelty of this research is the incorporation of Miura transformation constraints into neural networks to solve

nonlinear PDEs, which is an implementation method of unsupervised learning. The most noteworthy advantage of our method is that we can simply exploit the initial-boundary data of a solution of a certain nonlinear equation to obtain the data-driven solution of another evolution equation with the aid of Miura transformations and PINNs. In the process, the Miura transformation plays an indispensable role of a bridge between solutions of two separate equations. It is tailored to the inverse process of the Miura transformation and can overcome the difficulties in solving solutions based on the implicit expression. Moreover, two schemes are applied to perform abundant computational experiments to effectively reproduce dynamic behaviors of solutions for the well-known KdV equation and mKdV equation. Significantly, new data-driven solutions are successfully simulated and one of the most important results is the discovery of a new localized wave solution: kink-bell type solution of the defocusing mKdV equation and it has not been previously observed and reported to our knowledge. It provides a possibility for new types of numerical solutions by fully leveraging the many-to-one relationship between solutions before and after Miura transformations. Performance comparisons in different cases as well as advantages and disadvantages analysis of two schemes are also discussed. Based on the performance of two schemes and no free lunch theorem, they both have their own merits and thus more appropriate one should be chosen according to specific cases.

## **[04206] Drinfeld-Sokolov hierarchies and diagram automorphisms of affine Kac-Moody algebras**

**Format :** Talk at Waseda University

**Author(s) :** Chaozhong Wu (Sun Yat-Sen University)

**Abstract :** For a diagram automorphism of an affine Kac-Moody algebra such that the folded diagram is still an affine Dynkin diagram, we show that the associated Drinfeld-Sokolov hierarchy also admits an induced automorphism. We also show how to obtain the Drinfeld-Sokolov hierarchy associated to the affine Kac-Moody algebra that corresponds to the folded Dynkin diagram from the invariant sub-hierarchy of the original Drinfeld-Sokolov hierarchy. This is based on a joint work with Si-Qi Liu, Youjin Zhang and Xu Zhou.

02083 (2/3) : 4D @F309

## **[04907] On the long-time asymptotics of the modified Camassa-Holm equation in space-time solitonic regions**

**Format :** Online Talk on Zoom

**Author(s) :** Engui Fan (Fudan University)

**Abstract :** We study the long time asymptotic behavior for the Cauchy problem of the modified Camassa-Holm (mCH) equation in the solitonic regions. Our main technical tool is the representation of the Cauchy problem with an associated matrix Riemann-Hilbert (RH) problem and the consequent asymptotic analysis of this RH problem. Based on the spectral analysis of the Lax pair associated with the mCH equation and scattering matrix, the solution of the Cauchy problem is characterized via the solution of a RH problem in the new scale  $(y,t)$ . Further using the  $\partial$  generalization of the Deift-Zhou steepest descent method, we derive different long time asymptotic expansions of the solution  $u(y,t)$  in different space-time solitonic regions of  $\xi = y/t$ . We divide the half-plane  $\{(y,t) : -\infty < t < 0\}$  into four asymptotic regions: The phase function  $\Theta(z)$  has no stationary phase point on the jump contour in the space-time solitonic regions  $\xi \in (-\infty, -1/4) \cup (2, +\infty)$ , corresponding asymptotic approximations can be characterized with an  $N(\Lambda)$ -solitons with diverse residual error order  $O(t^{-1+2\rho})$ ; The phase function  $\Theta(z)$  has four phase points and eight phase points on the jump contour in the space-time solitonic regions  $\xi \in (0, 2)$  and  $\xi \in (-1/4, 0)$ , respectively. The corresponding asymptotic approximations can be characterized with an  $N(\Lambda)$ -soliton as well as an interaction term between soliton solutions and the dispersion term with diverse residual error order  $O(t^{-3/4})$ . Our results also confirm the soliton resolution conjecture and asymptotically stability of the  $N$ -soliton solutions for the mCH equation.

## **[05585] Local and global analyticity for a generalized Camassa-Holm system**

**Format :** Talk at Waseda University

**Author(s) :** Hideshi Yamane (Kwansei Gakuin University)

**Abstract :** We solve the analytic Cauchy problem for the generalized two-component Camassa-Holm system introduced by R. M. Chen and Y. Liu.

We show the existence of a unique local/global-in-time analytic solution under certain conditions.

This is the first result about global analyticity for a Camassa-Holm-like system.

The proof is based the technique by Barostichi, Himonas and Petronilho.

## [04390] Long-time asymptotics for the defocusing NLS equation with step-like boundary conditions

**Format :** Talk at Waseda University

**Author(s) :** Deng-Shan Wang (Beijing Normal University)

**Abstract :** The long-time asymptotics for the defocusing NLS equation with step-like boundary conditions is investigated by the Riemann-Hilbert formulation. Whitham modulation theory shows that there are six cases for this initial discontinuity problem according to the orders of the Riemann invariants. We formulate the leading-order terms and the corresponding error estimates for each region of the six cases by Deift-Zhou nonlinear steepest-descent method. It is demonstrated that the asymptotic solutions match very well with the results from Whitham modulation theory and the direct numerical simulations.

## [05490] New revival phenomena for bidirectional dispersive hyperbolic equations

**Format :** Talk at Waseda University

**Author(s) :** Jing Kang (Northwest University)

**Abstract :** In this talk, the dispersive revival and fractalisation phenomena for bidirectional dispersive equations on a bounded interval subject to periodic boundary conditions and discontinuous initial profiles are investigated. Firstly, we study the periodic initial-boundary problem of the linear beam equation with step function initial data, and analyze the manifestation of the revival phenomenon for the corresponding solutions at rational times. Next, we extend the investigation to the periodic initial-boundary problems of more general bidirectional dispersive equations. We prove that, if the initial functions are of bounded variation, the dynamical evolution of such periodic initial-boundary problem depend essentially upon the large wave number asymptotics of the associated dispersion relations. Integral polynomial or asymptotically integral polynomial dispersion relations produce dispersive revival/fractalisation rational/irrational dichotomy effects, whereas those with non-polynomial growth results in fractal profiles at all times. Finally, numerical experiments are used to demonstrate how such effects persist into the nonlinear regime, in the concrete case of the nonlinear beam equation. This is a joint work with Peter J. Olver, Xiaochuan Liu and Changzheng Qu.

02083 (3/3) : 4E @F309

## [05580] Darboux transformation and soliton solutions for a generalized Sasa-Satsuma equation

**Format :** Talk at Waseda University

**Author(s) :** Zuo-nong Zhu (Shanghai Jiao Tong University)Hongqian Sun (Shanghai Jiao Tong University)

**Abstract :** Sasa-Satsuma equation is an important integrable equation. In this talk, we will investigate a generalized Sasa-Satsuma equation introduced by Geng and Wu. Darboux transformation and soliton solutions including hump-type, breather-type solitons for the generalized Sasa-Satsuma equation are constructed.

## [05584] Rogue waves and solitons of nonlinear integrable/nearly integrable systems

**Format :** Talk at Waseda University

**Author(s) :** Zhenya Yan (Academy of Mathematics and Systems Science, Chinese Academy of Sciences)

**Abstract :** In this talk, we mainly discuss some properties of rogue waves and solitons of some nonlinear integrable/nearly integrable systems, which include stability, interactions and excitations of solitons, and rogue wave structures.

## [05579] The modified KdV equation on the background of elliptic function solutions

**Format :** Talk at Waseda University

**Author(s) :** Liming Ling (South China University of Technology)

**Abstract :** In this talk, we first introduce the spectral stability and orbital stability of the elliptic function solutions for the focusing modified Korteweg-de Vries (mKdV) equation with respect to subharmonic perturbations and construct the corresponding breather solutions to exhibit the unstable or stable dynamic behavior. On the other

hand, by using the Darboux-Backlund transformation, we construct multi-elliptic-localized wave solutions. The asymptotic analysis of these multi-elliptic-localized wave solutions is also involved in this talk.

## [04134] Pattern Transformation in Higher-Order Lumps of the Kadomtsev-Petviashvili I Equation

**Format :** Talk at Waseda University

**Author(s) :** Bo Yang (Ningbo University)

**Abstract :** Pattern formation in higher-order lumps of the Kadomtsev-Petviashvili I equation at large time is analytically studied. For a broad class of these higher-order lumps, we show that two types of solution patterns appear at large time. The first type of patterns comprises fundamental lumps arranged in triangular shapes, which are described analytically by root structures of the Yablonskii-Vorob'ev polynomials. As time evolves from large negative to large positive, this triangular pattern reverses itself along the x-direction. The second type of patterns comprise fundamental lumps arranged in non-triangular shapes in the outer region, which are described analytically by nonzero-root structures of the Wronskian-Hermit polynomials, together with possible fundamental lumps arranged in triangular shapes in the inner region, which are described analytically by root structures of the Yablonskii-Vorob'ev polynomials. When time evolves from large negative to large positive, the non-triangular pattern in the outer region switches its x and y directions, while the triangular pattern in the inner region, if it arises, reverses its direction along the x-axis. Our predicted patterns at large time are compared to true solutions, and excellent agreement is observed.

## [02109] Recent Advances on Numerical Analysis of Integral and Integro-differential Equations

**Session Time & Room :**

02109 (1/3) : 4C (Aug.24, 13:20-15:00) @E802

02109 (2/3) : 4D (Aug.24, 15:30-17:10) @E802

02109 (3/3) : 4E (Aug.24, 17:40-19:20) @E802

**Type :** Proposal of Minisymposium

**Abstract :** Since integral equations, integro-differential and nonlocal equations play an important role as mathematical models in science, engineering and finance, recent years have seen major developments in the design and analysis of efficient numerical methods for such equations. It is the aim of this minisymposium to bring together leading experts in these fields, in order to describe recent achievements and further communication between numerical analysts and computational scientists working on these problems.

**Organizer(s) :** Qiumei Huang, Hui Liang, Jiwei Zhang

**Classification :** 65R20, 65R30, Numerical Analysis of Integral and Integro-differential Equations

**Minisymposium Program :**

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02109 (1/3) : 4C @E802

## [02677] An hp-version of the discontinuous Galerkin method for fractional integro-differential equations with weakly singular kernels

**Format :** Talk at Waseda University

**Author(s) :** Yanping Chen (South China Normal University)

**Abstract :** In this talk, an hp-discontinuous Galerkin method is developed for the fractional integro-differential equations with weakly singular kernels. The key idea of our method is to first convert the fractional integro-differential equations into the Volterra integral equations, and then solve the equivalent integral equations using the hp-discontinuous Galerkin method. The prior error bounds for the proposed method are established in the L<sub>2</sub>-norm. Numerical results are presented to demonstrate the effectiveness of the proposed method.

## [03691] Implicitly Linear Jacobi Spectral-Collocation Methods for Weakly Singular Volterra-Hammerstein Integral Equations

**Format :** Talk at Waseda University

**Author(s) :** Qiumei Huang (Beijing University of Technology)Huitinh Yang (Beijing University of Technology)

**Abstract :** Weakly singular Volterra integral equations of the second kind typically have nonsmooth solutions near the initial point of the interval of integration, which seriously affects the accuracy of spectral methods. We present Jacobi spectral-collocation method to solve two-dimensional weakly singular Volterra-Hammerstein integral equations based on smoothing transformation and implicit linear method. The solution of the smoothed equation is much smoother than the original one after smoothing transformation and the spectral method can be used. For the Hammerstein nonlinear term, the implicitly linear method is applied to simplify the calculation and improve the accuracy. Convergence analysis in the  $L^\infty$ -norm is carried out and the exponential convergence rate is obtained. Finally, we demonstrate the efficiency of the proposed method by numerical examples.

## [03565] A collocation based approach for the numerical solution of singular fractional integro-differential equations

**Format :** Talk at Waseda University

**Author(s) :** Kaido Latt (University of Tartu)Arvet Pedas (University of Tartu)

**Abstract :** We consider a class of fractional integro-differential equations with certain type of singularities at the origin. We reformulate the original problem as a cordial Volterra integral equation and study the existence, uniqueness, and regularity of the exact solution. We also construct a collocation based numerical method for finding the approximate solution of the original problem and present some numerical examples.

## [02147] Solutions of second kind Fredholm integral equations by discrete projection methods

**Format :** Talk at Waseda University

**Author(s) :** Gobinda Rakshit (Rajiv Gandhi Institute of Petroleum Technology, Jais Campus, Amethi, Uttar Pradesh 229304)

**Abstract :** We are interested in approximate solutions of the integral equation  $x(s) - \int_0^1 \kappa(s, t, (x(t))dt = f(s)$ , where  $f$  and the kernel  $\kappa$  are given. A class of projection methods are available for obtaining approximate solutions to the above integral equation. Modified projection method is recently proposed and it exhibits higher orders of convergence as compared to the Galerkin/collocation (projection) methods. Here, we define and analyze a discrete version of the above projection methods.

02109 (2/3) : 4D @E802

## [03563] Numerical solution of fractional integro-differential equations

**Format :** Talk at Waseda University

**Author(s) :** Arvet Pedas (University of Tartu)Mikk Vikerpuur (University of Tartu)

**Abstract :** We consider a wide class of linear multi-term fractional integro-differential equations with Caputo derivatives and weakly singular kernels. First, we discuss the existence, uniqueness and smoothness of the exact solution. Then, using a suitable smoothing transformation and spline collocation techniques, we construct a high-order method for the numerical solution of the underlying problem. Finally, a numerical illustration of the proposed method is presented.

## [04175] A new linearized maximum principle preserving and energy stability scheme for the space fractional Allen-Cahn equation

**Format :** Talk at Waseda University

**Author(s) :** Yin Yang (Xiangtan University)Biao Zhang (Xiangtan University)

**Abstract :** In this talk, we present a new linearized two-level second-order scheme for the space fractional Allen-Cahn equation, which is based on the Crank-Nicolson method in time, second-order weighted and shifted Gr" unwald difference formula in space and Newton linearized technology to deal with nonlinear term. And we only need to solve a linear system at each time level. Then, the unique solvability of the scheme is given. Under the reasonable time step constraint, the discrete maximum principle, energy stability and error analysis are also studied. At last, some numerical experiments show that the proposed method is reasonable and effective.

## [03914] High accuracy analysis of FEMs for several time-fractional PDEs

**Format :** Talk at Waseda University

**Author(s) :** Yanmin Zhao (Xuchang University)

**Abstract :** In this talk, convergence and superconvergence analysis for several kinds of time-fractional partial differential equations will be discussed by use of finite element methods and proper finite difference schemes. At the same time, unconditional stability properties of fully-discrete schemes are presented. Moreover, numerical experiments are provided to confirm the theoretical results. And, some relevant topics are included.

## [02240] Discontinuous piecewise polynomial collocation methods for integral-algebraic equations of Hessenberg type

**Format :** Talk at Waseda University

**Author(s) :** Hui Liang (Harbin Institute of Technology, Shenzhen) Hecong Gao (Harbin Institute of Technology, Shenzhen)

**Abstract :** We mainly consider the integral-algebraic equations of Hessenberg type. The tractability index is investigated. The existence, uniqueness, and regularity are analyzed, and the resolvent representation is given. First, the convergence theory of perturbed collocation methods in discontinuous piecewise polynomial space is established for first-kind Volterra integral equations, then it is used to derive the optimal convergence properties of discontinuous piecewise polynomial collocation methods for Hessenberg-type integral-algebraic equations. Numerical examples illustrate the theoretical results.

02109 (3/3) : 4E @E802

## [04726] Mean square exponential stability and practical mean square exponential stability of stochastic delay differential equations driven by G-Brownian motion and Euler-Maruyama approximations

**Format :** Online Talk on Zoom

**Author(s) :** Haiyan Yuan (Heilongjiang institute of technology)

**Abstract :** This paper investigates the mean-square (MS) exponential stability and the practical mean square (PMS) exponential stability of stochastic delay differential equations driven by G-Brownian motion (G-SDDEs) and the numerical solution generated by Euler-Maruyama (EM) method. We present a weaker condition to prove the MS exponential stability of G-SDDEs instead of choosing a Lyapunov function under the case that the origin is an equilibrium point. In order to study whether the performance of G-SDDEs near an unstable equilibrium point is acceptable, we introduce the practical stability and establish a new generalized Gronwall inequality based on which we prove the PMS exponential stability of G-SDDEs. We also study the numerical approximations for G-SDDEs. We first establish the stability equivalence between the discrete EM method and the continuous EM method, then we prove that the continuous EM method can reproduce the MS exponential stability and the PMS exponential stability of G-SDDEs under some restrictions on the step size. Furthermore, two numerical experiments are conducted to confirm our theoretical results.

## [02676] Superconvergent postprocessing of the continuous and discontinuous Galerkin methods for nonlinear Volterra integro-differential equations

**Format :** Online Talk on Zoom

**Author(s) :** Lijun Yi (Shanghai Normal University) Mingzhu Zhang (Shanghai Normal University)

**Abstract :** In this talk, we introduce novel postprocessing techniques for improving the accuracy of the CG and DG methods for nonlinear Volterra integro-differential equations. We first show that the CG and DG method superconverge at the nodal points of the time partition. We further prove that the postprocessed CG and DG approximations converge one order faster than the unprocessed CG and DG approximations in the  $L^2$ -,  $H^1$ - and  $L^\infty$ -norms. As a by-product of the postprocessed superconvergence results, we construct several a posteriori error estimators and prove that they are asymptotically exact. Numerical examples are presented to verify the theoretical results.

# [02115] Theory and applications of random/non-autonomous dynamical systems Part III

**Session Time & Room :** 5B (Aug.25, 10:40-12:20) @F309

**Type :** Proposal of Minisymposium

**Abstract :** Dynamical systems evolving in the existence of noise, is called random dynamical systems. The basic properties, such as stability, bifurcation, and statistical properties, of such random or non-autonomous dynamical systems have not been well studied in mathematics and physics. Recently, cooperative research on random dynamical systems has been developed in the fields in statistical and nonlinear physics, dynamical system theory, ergodic theory, and stochastic process theory. In this mini-symposium, we consider theory and applications of random dynamical systems. In Part III, we discuss infinite ergodicity and random dynamical systems.

**Organizer(s) :** Hiroki Sumi, Yuzuru Sato, Kouji Yano, Takuma Akimoto

**Classification :** 37H05, 37A50, 37A05, 37H12

**Minisymposium Program :**

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02115 (1/1) : 5B @F309 [Chair: Kouji Yano]

## [04171] Arcsine and Darling--Kac laws for piecewise linear random interval maps

**Format :** Talk at Waseda University

**Author(s) :** Kouji Yano (Osaka University)

**Abstract :** We give examples of piecewise linear random interval maps satisfying arcsine and Darling--Kac laws, which are analogous to Thaler's arcsine and Aaronson's Darling--Kac laws for the Boole transformation. They are constructed by random switch of two piecewise linear maps with attracting or repelling fixed points, which behave as if they were indifferent fixed points of a deterministic map.

## [04000] Generalized uniform laws for occupation times of intermittent maps

**Format :** Talk at Waseda University

**Author(s) :** Toru Sera (Osaka University)

**Abstract :** Interval maps with indifferent fixed points are called intermittent maps. In this talk, we impose the condition that the orbit stays away from indifferent fixed points at the final observation time. Under this condition, we study the scaling limit of occupation times. This talk is based on joint work with Jon. Aaronson (Tel Aviv).

## [04085] Estimates of invariant measures for random maps

**Format :** Talk at Waseda University

**Author(s) :** Tomoki Inoue (Ehime University)

**Abstract :** We consider a random dynamical system such that one transformation is randomly selected from a family of transformations and then applied on each iteration. Especially, we consider random dynamical systems with indifferent fixed points and/or with unbounded derivatives. Under some conditions, such random dynamical systems have absolutely continuous invariant measures. We give some estimates of the absolutely continuous invariant measures.

## [04503] probability and ergodic theory for inner functions

**Format :** Talk at Waseda University

**Author(s) :** jon aaronson (tel aviv university)Kouji Yano (Osaka University)

**Abstract :** An analytic endomorphism of the unit disk is called an inner function if its boundary limit defines a transformation of

the circle - which is necessarily Lebesgue nonsingular. I'll review the ergodic theory of inner functions & present some

results recently obtained with Mahendra Nadkarni.

part\_2

# [02130] Fluid-structure interactions in geophysical flows

**Session Time & Room :**

02130 (1/2) : 4D (Aug.24, 15:30-17:10) @E820

02130 (2/2) : 4E (Aug.24, 17:40-19:20) @E820

**Type :** Proposal of Minisymposium

**Abstract :** Fluid-structure interactions appear on many different scales of our planet. For example, centimeter-scale pebble stones are shaped by flow erosion, while kilometer-scale karst terrains are a result of dissolution. Even the planetary-scale plate tectonics are believed to be driven by the convection in Earth's mantle. In this minisymposium, we focus on lab-scale experiments and math modeling of such geophysical fluid-structure interactions, exploring the connections between processes like convection, erosion, dissolution, and melting. With a diverse group of speakers, this minisymposium will initiate a new and combined effort to address these important geophysical phenomena.

**Organizer(s) :** Jinzi Mac Huang, Nick Moore

**Classification :** 76-05, 76-10

**Minisymposium Program :**

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02130 (1/2) : 4D @E820 [Chair: Jinzi Mac Huang]

## [04348] How Fluid-Mechanical Erosion Creates Anisotropic Porous Media

**Format :** Talk at Waseda University

**Author(s) :** Bryan Quaife (Florida State University)Nick Moore (Colgate University)Jake Cherry (Florida State University)Shang-Huan Chiu (Lehigh University)

**Abstract :** When a porous medium erodes, microscopic changes of the grain morphology give rise to larger-scale features such as channelization. Using a boundary integral formulation, we characterize these changes by simulating erosion of porous media. A Cauchy-integral formulation and associated quadrature formulas enable us to resolve dense configurations of nearly contacting bodies. We observe that substantial anisotropy develops over the course of erosion; that is, the configurations that result from erosion permit flow in the longitudinal direction more easily than in the transverse direction by up to a factor of six. These results suggest that the erosion of solid material from groundwater flows may contribute to previously observed anisotropy of natural porous media.

## [04569] Moving boundaries in thermal convection

**Format :** Talk at Waseda University

**Author(s) :** Jun Zhang (New York University)

**Abstract :** With simple experiments, we study how mobile boundaries interact with thermally convective flows. When turbulence intensity in thermal convection is sufficiently large, flow patterns are random. However, if a mobile boundary is added to the system, and allowed to freely interact with the surrounding flows, the structure-fluid system may show orderly behaviors, and the flow patterns also become more regular. Geophysical motivations and potential applications will also be discussed in this talk.

## [04835] Using asymptotic analysis to improve numerical methods for multiphase flows

**Format :** Talk at Waseda University

**Author(s) :** Eric William Hester (UCLA)Andrea Bertozzi (UCLA)

**Abstract :** Diffuse-interface methods approximate discontinuous boundary conditions with smooth source terms - avoiding the need to explicitly discretise multiphase interfaces. But this approximation only converges in the limit. Using the signed-distance function I will outline a general framework for the asymptotic analysis of diffuse-interface methods. I will thereby optimise diffuse-interface simulations of fluid-structure interaction, melting and dissolving ocean icebergs, and dynamic contact lines in three-phase fluids.

## [04665] Laser shot on water and ice

**Format :** Online Talk on Zoom

**Author(s) :** Daosheng Deng (Fudan University)

**Abstract :** The strong interaction between laser and ice or water, arising from the strong photothermal effect, can lead the diverse intriguing phenomena. This talk will present the dancing bubble generated in water by laser, and report the melting of ice under the laser illumination.

02130 (2/2) : 4E @E820 [Chair: Jun Zhang]

## [04383] A simple model on what drives continental drifts

**Format :** Talk at Waseda University

**Author(s) :** Jinzi Mac Huang (New York University Shanghai)

**Abstract :** It is well known that the continents of earth do not stay in place, and thermal convection in Earth's mantle is believed to be the driving force of these motions. How does mantle convection couple to the continental drift? Does the moving continent affect the mantle motion beneath it? We address these questions through a simple fluid-structure interaction model, exploring the fluid mechanical origin of continental drift and the possibility of modeling tectonic plate interactions.

## [05512] Computing the diffusivity of a particle subject to dry friction with colored noise

**Format :** Talk at Waseda University

**Author(s) :** Laurent Mertz (City University of Hong Kong)Josselin Garnier (Polytechnique)

**Abstract :** Experimental studies and numerical simulations have been devoted to the motion of an object subjected to a dry friction and an external random force. The experimental and numerical observations suggest that the variance of the object displacement grows linearly with time. Here, the variance growth rate is called diffusivity. The goal of this paper is to propose efficient stochastic simulation methods for computing the diffusivity when the external random force is white or colored noise.

## [04815] The Formation of Karst Pinnacles

**Format :** Online Talk on Zoom

**Author(s) :** Nick Moore (Colgate University)

**Abstract :** Recent experiments demonstrate how dissolution, in conjunction with gravitationally-induced convective flows, can create sharp geometric features. These laboratory-created structures give insight into geological features known as karst pinnacles. A new computational approach reveals convergence to a morphological attractor with high, yet finite, tip curvature. These results reverse previous hypotheses on shock formation (i.e. finite-time blowup of tip curvature), agree well with laboratory experiments, and enable simple estimates for the age of geological structures.

## [02154] Hypergeometric functions in statistics and particle physics

**Session Time & Room :**

02154 (1/2) : 3C (Aug.23, 13:20-15:00) @G305

02154 (2/2) : 3D (Aug.23, 15:30-17:10) @G305

**Type :** Proposal of Minisymposium

**Abstract :** Recent years have shed new light on the theory of hypergeometric functions.

They appear as marginal likelihood integrals in statistics and as Feynman integrals in quantum field theory.

Evaluating these integrals is a central, but challenging problem in these areas.

Advances in algebraic methods provides new insights into this problem.

Such methods rest on graph theory, combinatorics of convex bodies, Gröbner bases, D-modules, and toric geometry, to name a few.

These new perspectives also raise fascinating new questions, both theoretical and computational.  
We gather active researchers in this area to identify such questions, and to accelerate the progress.

**Organizer(s)** : Saiei-Jaeyeong Matsubara-Heo, Nobuki Takayama

**Classification** : 14F10, 16Z05, 62R01, 81T18, 33C70

**Minisymposium Program :**

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02154 (1/2) : 3C @G305

## [03807] Towards Algebraic Analysis of Hypergeometric Systems

**Author(s)** : Saiei-Jaeyeong Matsubara-Heo (Kumamoto University)

**Abstract** : A hypergeometric function is an analytic function defined in terms of an elementary integral. A hypergeometric system is a system of differential (or difference) equations that it satisfies, which ties analysis to various fields of algebra, such as ring/module theory (D-modules), homological algebra, or combinatorics of polytopes. This talk aims to provide the speaker's view on the current state of the art. A unifying thread is a study of algebraic equations.

## [03843] D-Module Techniques for Solving Differential Equations in the Context of Feynman Integrals

**Author(s)** : Anna-Laura Sattelberger (Department of Mathematics, KTH Royal Institute of Technology)

**Abstract** : I explain how to compute series solutions of regular holonomic D-ideals with Gröbner basis methods via an algorithm due to Saito, Sturmfels, and Takayama. As a point in case, I consider a D-ideal originating from a triangle Feynman diagram. This talk is based on joint work (arXiv:2303.11105) with Johannes Henn, Elizabeth Pratt, and Simone Zoia. Therein, we compare D-module techniques to dedicated methods developed for solving differential equations in the context of Feynman integrals.

## [04120] Distribution of eigenvalues of a singular elliptical Wishart matrix

**Author(s)** : Koki Shimizu (Tokyo University of Science) Hiroki Hashiguchi (Tokyo University of Science)

**Abstract** : We derive the exact distributions of eigenvalues of a singular Wishart matrix under the elliptical model. These distributions cover the results under the Gaussian model as a special case. The joint density of eigenvalues and distribution function of the largest eigenvalue for a singular elliptical Wishart matrix are represented in terms of generalized hypergeometric functions. Numerical computations for the distribution of the largest eigenvalue are conducted under Gaussian and Kotz-type models.

## [04121] Restriction algorithms for holonomic systems and their applications

**Author(s)** : Nobuki Takayama (Kobe University)

**Abstract** : Definite integrals with parameters (in statistics and physics) satisfy holonomic systems (maximally overdetermined systems of linear PDEs). When parameters are restricted to an algebraic set, these integrals satisfy smaller or simpler holonomic systems. We will survey algorithms of finding these smaller or simpler systems with applications and numerical examples.

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02154 (2/2) : 3D @G305

## [04146] Twisted cohomology and likelihood ideals

**Author(s)** : Simon Telen (MPI MiS Leipzig) Saiei-Jaeyeong Matsubara-Heo (Kumamoto University)

**Abstract** : A likelihood function on a smooth very affine variety gives rise to a twisted de Rham complex. We show how its top cohomology vector space degenerates to the coordinate ring of the critical points defined by the likelihood equations. We obtain a basis for cohomology from a basis of this coordinate ring. We investigate the dual picture, where twisted cycles correspond to critical points. We show how to expand a twisted cocycle in terms of a basis, and apply our methods to Feynman integrals from physics.

## [04152] Algebraic A-hypergeometric Laurent series and residues

**Author(s)** : Alicia Dickenstein (University of Buenos Aires)

**Abstract** : A-hypergeometric systems of partial differential equations (introduced by Gelfand, Kapranov and Zelevinsky) have natural geometric solutions, with singularities on the associated discriminant. We describe A-hypergeometric algebraic Laurent series associated with Cayley configurations of  $n$  lattice configurations in  $n$  space. These algebraic series are generated by certain combinatorially defined sums of point residues, whose computation can be interpreted in terms of a toric degeneration. Joint work with E. Cattani and F. Martinez.

## [04334] Sampling from toric models and hypergeometric functions

**Author(s)** : Shuhei Mano (The Institute of Statistical Mathematics)

**Abstract** : The toric model is an important class of stochastic models, and sampling from toric models has various applications including statistics. The sampling problem is related with hypergeometric functions, because the normalizing constant of the probability function is a multi-variable polynomial and satisfies a GKZ-hypergeometric system. In this talk, I will review several problems in which the relationship works effectively.

# [02163] Recent Developments in Stochastic Numerics and Computational Finance

**Session Time & Room :**

02163 (1/3) : 4C (Aug.24, 13:20-15:00) @E505

02163 (2/3) : 4D (Aug.24, 15:30-17:10) @E505

02163 (3/3) : 4E (Aug.24, 17:40-19:20) @E505

**Type** : Proposal of Minisymposium

**Abstract** : Stochastic numerical analysis becomes so important in probability theory, statistics and applied mathematics especially in machine learning and data science and achieves a great success in computational finance. The aim of the minisymposium is to highlight recent developments in stochastic numerical analysis and computational finance, and to interact with researchers working on the fields. Topics will include deep learning methods for stochastic differential equations and PDEs, new computational methods for pricing derivatives, portfolio optimization and risk management, and their theoretical analysis.

**Organizer(s)** : Jiro Akahori, Shioiti Ninomiya, Toshihiro Yamada

**Classification** : 65C05, 65C10, 65C20, 65C30, 91G60

**Minisymposium Program :**

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02163 (1/3) : 4C @E505 [Chair: Yuji Shinozaki]

## [03032] Policy improvement algorithm for an optimal consumption and investment problem under general stochastic factor models

**Format** : Talk at Waseda University

**Author(s)** : Kazuhiro Yasuda (Hosei university)Hiroaki Hata (Hitotsubashi university)

**Abstract** : In this talk, we propose a policy improvement algorithm for a consumption and investment problem on a finite time horizon to optimize a discounted expected power utility of consumption and terminal wealth. We employ a general stochastic factor model which means that the returns and volatilities of assets are random and affected by some economic factors, modeled as diffusion processes. We establish an iteration procedure converging to the value function and the optimal strategies obtained in Hata, Nagai and Sheu (2018). Some numerical results are shown to understand convergence behaviors of the algorithm.

**[03381] Growth in Fund Models****Format :** Talk at Waseda University**Author(s) :** Hyeng Keun Koo (Ajou University)Constantinos Kardaras (London School of Economics)Johannes Ruf (London School of Economics)**Abstract :** We study estimation of growth in fund models, i.e., statistical descriptions of markets where all asset returns are spanned by the returns of a lower-dimensional collection of funds, modulo orthogonal noise. The loss of growth due to estimation error in fund models under local frequentist estimation is determined entirely by the number of funds. A shrinkage method that targets maximal growth with the least amount of deviation is proposed.**[03015] Carbon Emissions Pricing by Forward and Double Barrier Backward SDE approach****Format :** Talk at Waseda University**Author(s) :** Tadashi Hayashi (Mitsubishi UFJ Trust and Banking Corporation)**Abstract :** Under the circumstances of global warming caused by increasing in greenhouse gases, there are many theoretical and empirical studies in carbon emissions to control and reduce the gases. Our study is focused on the carbon emissions pricing via Forward and Double Barrier BSDE as another pricing approach. This modelling would be a new approach of carbon emissions pricing and therefore lead to a new chance of empirical simulation.**[03307] Irreversible consumption habit under ambiguity: singular control and optimal G-stopping time****Format :** Talk at Waseda University**Author(s) :** Kyunghyun Park (Nanyang Technological University)HOI YING WONG (The Chinese University of Hong Kong )Kexin Chen (The Hong Kong Polytechnic University)**Abstract :** Consider robust utility maximization with an irreversible consumption habit, where an agent concerned about model ambiguity is unwilling to decrease consumption and must simultaneously contend with a disutility (i.e., an adjustment cost) due to a consumption increase. While the optimization is a robust analog of singular control problems over a class of consumption-investment strategies and a set of probability measures, it is a new formulation that involves non-dominated probability measures of the diffusion process for the underlying assets in addition to singular controls with an adjustment cost. This paper provides a novel connection between the singular controls in the optimization and the optimal  $G$ -stopping times in a  $G$ -expectation space, using a duality theory. This connection enables to derive the robust consumption strategy as a running maximum of the stochastic boundary, which is characterized by a free boundary arising from the optimal  $G$ -stopping times. The duality, which relies on arguments based on reflected  $G$ -BSDEs, is achieved by verifying the first-order optimality conditions for the singular control, the budget constraint equation for the robust strategies, and the worst-case realization under the non-dominated measures.

02163 (2/3) : 4D @E505 [Chair: Toshihiro Yamada]

**[03674] New deep NN architecture using higher-order weak approximation****Format :** Talk at Waseda University**Author(s) :** Syoiti Ninomiya (Tokyo Institute of Technology)Yuming MA (Tokyo Institute of Technology)**Abstract :** New deep learning neural networks based on high-order weak approximation algorithms for stochastic differential equations are proposed. The behavior of these new algorithms when applied to the problem of pricing financial derivatives is also reported. The architectural key to the deep learning neural network proposed here is a high-order discretization method of Runge-Kutta type, in which the weak approximation of stochastic differential equations is realized by iterative substitutions and their linear summation.

## [03488] A higher order discretization scheme for backward stochastic differential equations combined with a non-linear discrete Clark-Ocone formula

**Format :** Talk at Waseda University

**Author(s) :** Kaori Okuma (Ritsumeikan University)

**Abstract :** In this talk, the author first introduces a discretization scheme of arbitrary order for backward stochastic differential equations. Then, by establishing a mathematical algorithm based on a non-linear discrete Clark-Ocone formula, which was previously established by the author and her collaborators, the author claims that the scheme is potentially implementable in a “deep solver” type numerical algorithm — a scheme using approximation by deep neural networks and stochastic gradient descent — for a semi-linear partial differential equation.

## [03622] New deep learning-based algorithms for high-dimensional Bermudan option pricing

**Format :** Talk at Waseda University

**Author(s) :** Riu Naito (Hitotsubashi University) Toshihiro Yamada (Hitotsubashi University)

**Abstract :** In this talk, we introduce efficient algorithms for pricing high-dimensional Bermudan options. The proposed methods provide an accurate approximation for Bermudan options by discretizing the interval of early-exercise dates with weak approximation schemes for stochastic differential equations. The deep learning-based approximation for conditional expectations at each exercise date works well for high-dimensional problems compared to the least squares Monte Carlo method. Numerical experiments confirm the validity of the methods.

## [05412] On-Policy and Off-Policy q-Learning in Continuous Time

**Format :** Talk at Waseda University

**Author(s) :** Yanwei Jia (Chinese University of Hong Kong) Xunyu Zhou (Columbia University)

**Abstract :** We study the continuous-time counterpart of Q-learning for reinforcement learning (RL) under the entropy-regularized, exploratory formulation introduced by Wang et al (2020). As the conventional (big) Q-function collapses in continuous

time, we consider its first-order approximation and coin the term (little) q-function". This function is related to the instantaneous advantage rate function as well as the Hamiltonian. We develop aq-learning" theory around the

q-function that is independent of time discretization. Given a stochastic policy, we jointly characterize the associated q-function and value function by martingale conditions of certain stochastic processes, in both on-policy and off-policy

settings. We then apply the theory to devise different actor-critic algorithms for solving underlying RL problems, depending on whether or not the density function of the Gibbs measure generated from the q-function can be computed explicitly.

02163 (3/3) : 4E @E505 [Chair: Kazuhiro Yasuda]

## [03150] An Approximation Scheme for Path-Dependent BSDEs

**Format :** Talk at Waseda University

**Author(s) :** Hyungbin Park (Seoul National University) Ji-Uk Jang (Seoul National University)

**Abstract :** In this work, we study an approximation scheme for solutions to forward-backward stochastic differential equations (FBSDEs) with non-anticipative coefficients. When the non-anticipative coefficients have Fréchet derivatives or can be approximated by non-anticipative functionals having Fréchet derivatives, we show the Picard-type iteration converges to the FBDSE solution and provide its convergence rate. Using this result, we establish a numerical method for solutions of second-order parabolic path-dependent partial differential equations. To achieve this, weak approximation of martingale representation theorem (Cont, Rama, and Yi Lu. “Weak approximation of martingale representations.” Stochastic Processes and their Applications 2016) is employed. Our results generalize the scheme for Markovian cases in (Bender, Christian, and Robert Denk. “A forward scheme for backward SDEs.” Stochastic processes and their applications, 2007)

## [03659] Practical high-order recombination algorithms for weak approximation of stochastic differential equations : Recursive patch dividing and its effects to singularities of terminal conditions

**Format :** Talk at Waseda University

**Author(s) :** Syoiti Ninomiya (Tokyo Institute of Technology)Yuji Shinozaki (Bank of Japan)

**Abstract :** This study proposes practically feasible implementation algorithms of the high-order recombination to apply to the weak approximation problem of SDEs, by extending and refining the work of Lyons and Litterer(2012). Specifically, new recursive patch dividing algorithms, which are based on the refined patch radius criteria, are proposed. Our numerical experiments demonstrate that the new recursive patch dividing algorithms are still efficient even when the terminal condition  $f$  becomes more singular.

## [03645] Extended Milstein scheme for hypoelliptic diffusions

**Format :** Talk at Waseda University

**Author(s) :** Yuga Iguchi (University College London)Toshihiro Yamada (Hitotsubashi University)

**Abstract :** For a wide class of diffusion processes, precisely hypoelliptic diffusions, we propose an effective and simple numerical scheme as an extension of Milstein scheme that outperforms Euler-Maruyama (EM) scheme (and standard Milstein scheme), though they share the same convergence rate in a weak sense. Analytic error term for the new scheme is derived and compared with that for EM scheme under non-smooth test functions. The effectiveness of the proposed scheme is also shown through numerical experiments for hypoelliptic diffusions appearing in finance.

## [03489] Wong-Zakai approximation for stochastic PDEs and HJM model

**Format :** Talk at Waseda University

**Author(s) :** TOSHIYUKI NAKAYAMA (MUFG Bank, Ltd.)

**Abstract :** We talk about semi-linear stochastic differential equation (SPDE) driven by a finite dimensional Brownian motion.

$$dX(t) = (AX(t) + b(X(t)))dt + \sum_{j=1}^r \sigma_j(X(t))dB^j(t), \quad X(0) = x_0.$$

Our goal is to establish a convergence rate with the generator  $A$  which is allowed to be the infinitesimal generator of an arbitrary strongly continuous semigroup.

Finally, we will introduce an application example for SPDE called HJMM that appears in mathematical finance. This talk is based on a co-authored paper with Stefan Tappe.

## [02169] Recent advances on numerical methods for stochastic ordinary differential equations

**Session Time & Room :**

02169 (1/2) : 1E (Aug.21, 17:40-19:20) @E506

02169 (2/2) : 2C (Aug.22, 13:20-15:00) @E506

**Type :** Proposal of Minisymposium

**Abstract :** Stochastic differential equations appear nowadays as a modeling tool in many branches of science and industry as finance, biology, and mean field theory, etc. Numerical methods play a key role in understanding and exploring the dynamics of stochastic differential equations. Some new challenges arise from real-world applications, for example, a stochastic model with non-globally Lipschitz diffusion, singular initial value problems with white noises, mean-field interactions, or the positivity preserving property. The aim of this minisymposium is to bring the researchers in these fields together to discuss recent advances and influence more collaborations.

**Organizer(s) :** Qian Guo, Wanrong Cao, Hongjiong Tian, Liangjian Hu

**Classification :** 65C30

**Minisymposium Program :**

## [03230] Deterministic implicit two-step Milstein methods for stochastic differential equations

**Format :** Talk at Waseda University

**Author(s) :** Hongjiang Tian (Shanghai Normal University)Quanwei Ren (Henan University of Technology)Tianhai Tian (Monash University)

**Abstract :** We propose a class of deterministic implicit two-step Milstein methods for solving Itô stochastic differential equations. Theoretical analysis is conducted for the convergence and stability properties of the proposed methods. We derive sufficient conditions such that these methods have the mean-square(M-S) convergence of order one, as well as sufficient and necessary conditions for linear M-S stability of the implicit two-step Milstein methods. Stability analysis shows that our proposed implicit two-step Milstein methods have much better stability property than those of the corresponding two-step explicit or semi-implicit Milstein methods. Numerical results are presented to confirm our theoretical analysis results.

## [03158] Numerical methods for stochastic singular initial value problems

**Format :** Online Talk on Zoom

**Author(s) :** Nan Deng (Southeast University)Wanrong Cao (Southeast University)Guofei Pang (Southeast University)

**Abstract :** In this work, we investigate the strong convergence of the Euler-Maruyama method for second-order stochastic singular initial value problems with additive white noise. The singularity at the origin brings a big challenge that the classical framework for stochastic differential equations and numerical schemes cannot work. By converting the problem to a first-order stochastic singular differential system, the existence and uniqueness of the exact solution is studied. Moreover, under some suitable assumptions, it is proved that the Euler-Maruyama scheme is of  $(1/2 - \epsilon)$  order convergence in mean-square sense, where  $\epsilon$  is an arbitrary small positive number, which is different from the consensus that the Euler-Maruyama method is convergent with first order in strong sense when solving stochastic differential equations with additive white noise. While, it is found that if the diffusion coefficient vanishes at the origin, the convergent order in mean-square sense will be raised to  $1 - \epsilon$ . Our theoretical findings are well verified by numerical examples.

## [03262] A Positivity Preserving Lamperti Transformed Euler-Maruyama Method for Solving the Stochastic Lotka-Volterra Competition Model

**Format :** Online Talk on Zoom

**Author(s) :** Yan Li (Southeast university)Wanrong Cao (Southeast University)

**Abstract :** A new positivity preserving numerical scheme is presented for a class of d-dimensional stochastic Lotka-Volterra competitive models, which are characterized by super-linear coefficients and positive solutions. The scheme, dubbed the Lamperti transformed Euler-Maruyama method, approximates the exact solution by integrating a Lamperti-type transformation with an explicit Euler-Maruyama method that has the benefit of being explicit and straightforward to implement. Even though the coefficients of the transformed models grow exponentially and do not satisfy the general monotonicity condition, based on the exponential integrability of the solution, it is proved that the proposed numerical method is of  $1/2$ -order strong convergence. In particular, when matrix A of the model is a diagonal matrix, the first-order strong convergence is also obtained. Without any step size constraints, the method can preserve long-time dynamical properties such as extinction and pth moment exponential asymptotic stability. Numerical examples are given to support our theoretical conclusions.

## [03037] Convergence rate in $L^p$ sense of tamed EM scheme for highly nonlinear neutral multiple-delay stochastic McKean-Vlasov equations

**Format :** Online Talk on Zoom

**Author(s) :** Shuaibin Gao (Shanghai Normal University)Qian Guo (Shanghai Normal University)Junhao Hu (South-Central University For Nationalities)Chenggui Yuan (Swansea University)

**Abstract :** This paper focuses on the numerical scheme of highly nonlinear neutral multiple-delay stochastic McKean-Vlasov equation (NMSMVE) by virtue of the stochastic particle method. First, under general assumptions, the results about propagation of chaos in  $L^p$  sense are shown. Then the tamed Euler-Maruyama scheme to the corresponding particle system is established and the convergence rate in  $L^p$  sense is obtained. Furthermore, combining these two results gives the convergence error between the objective NMSMVE and numerical

approximation, which is related to the particle number and step size. Finally, two numerical examples are provided to support the finding.

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02169 (2/2) : 2C @E506

## [02178] Efficient computational methods for data matrices: exploiting sparsity and structure

**Session Time & Room :**

02178 (1/2) : 5B (Aug.25, 10:40-12:20) @E508

02178 (2/2) : 5C (Aug.25, 13:20-15:00) @E508

**Type :** Proposal of Minisymposium

**Abstract :** This mini-symposium focuses on new applications from data analysis where sparse and structured matrices arise, as opposed to well-studied applications in scientific and engineering simulation. In addition to these new applications, we shall highlight algorithmic advances for these objects with a focus on techniques like randomisation, parallelisation, and use of modern computer hardware. The overall goal of this gathering is to help researchers see connections among these newer data-driven application areas and identify new computational building blocks that might benefit multiple domains.

**Organizer(s) :** Richard Vuduc, Srinivas Eswar  
**Sponsor :** This session is sponsored by the SIAM Activity Group on Supercomputing.

**Classification :** 65F50, 65F55, 68W10, 68W20

**Minisymposium Program :**

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02178 (1/2) : 5B @E508 [Chair: Richard Vuduc]

## [04733] Structured Matrices in Unsupervised Cross-Validation

**Format :** Talk at Waseda University

**Author(s) :** Srinivas Eswar (Argonne National Laboratory)

**Abstract :** We consider matrix low-rank approximation algorithms in the setting of unsupervised cross-validation. Unlike most structured matrix computations, a cross-validation user has more control of sparsity, with different choices implying different performance trade-offs. For example, controlling the rank of these matrices results in a trade-off between efficiency and cross-validation accuracy. This talk surveys these choices and trade-offs. Additionally, this presentation will also introduce the minisymposium.

## [04283] Randomized Algorithms for Rank Structured Matrices

**Format :** Talk at Waseda University

**Author(s) :** Per-Gunnar Martinsson (University of Texas at Austin)

**Abstract :** The talk describes randomized algorithms for computing a data sparse representation of a rank structured matrix (HSS, HODLR, H-matrix, ...). The algorithms are black box in that they interact with the target matrix only through its action on vectors, making them ideal for tasks such as forming Schur complements or matrix matrix multiplication. When the target matrix can be applied in O(N) operations, the compression as a whole typically has linear complexity as well.

## [03473] Scalable Data Analytics using Sparse Matrices

**Format :** Talk at Waseda University

**Author(s) :** Giulia Guidi (Cornell University)

**Abstract :** Massively parallel systems are vital for processing large data and play a critical role in data analysis. However, programming high-performance computing systems poses productivity and scalability challenges. Here, we focus here on advances in genome sequencing and the associated flood of genomic data, which present computational challenges and require new approaches.

This work demonstrates the feasibility of writing parallel code for irregular genomic computation through sparse matrix abstraction for de novo long-read genome assembly.

## [04632] Structure of Fisher information matrices in deep learning

**Format :** Talk at Waseda University

**Author(s) :** Rio Yokota (Tokyo Institute of Technology)

**Abstract :** Fisher information matrices have many applications in deep learning such as continual learning, generalization metrics, hyperparameter prediction, model sparsification, and optimization. The Fisher information matrix has a Kronecker product structure, which can be exploited to accelerate its computation. This talk will cover the various applications of Fisher information matrices, and its relation to Hessian and Gauss-Newton matrices, along with the theory behind its approximation through Kronecker factorization.

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02178 (2/2) : 5C @E508 [Chair: Srinivas Eswar]

## [04795] Exploiting Supernodal Structures in Sparse All Pair Shortest Path Computation.

**Format :** Talk at Waseda University

**Author(s) :** Piyush K Sao (Oak Ridge National Laboratory)Prasun Gera (cerebras)Hao Lu (Oak Ridge National Laboratory)Ramki Kannan (Oak Ridge National Laboratory)Richard W Vuduc (Georgia Institute of Technology)Thomas Potok (Oak Ridge National Laboratory)

**Abstract :** We introduce a novel approach for efficiently solving all-pairs shortest path problems on sparse graphs. We leverage the techniques from sparse Cholesky factorization, including fill-in-reducing ordering, supernodal traversal, and elimination tree parallelism for APSP computation. Our method uses semi-ring notation to express graph algorithms in linear algebraic form and employs BLAS level-III semi-ring operations. Our parallel prototype implementation significantly outperforms a non-sparsity-exploiting Floyd-Warshall algorithm and competes with Dijkstra's algorithm for specific sparse graph classes.

## [04585] Optimizations of H-matirx-vector Multiplication for Many-core Processors

**Format :** Talk at Waseda University

**Author(s) :** Tetsuya Hoshino (Nagoya University)Akihiro Ida (Japan Agency for Marine-Earth Science and Technology)Toshihiro Hanawa (The University of Tokyo)

**Abstract :** Hierarchical matrices (H-matrices) can robustly approximate the dense matrices that appear in the boundary element method (BEM). To accelerate the solving of linear systems in the BEM, we must speed up hierarchical matrix–vector multiplication (HiMV). This presentation discusses optimization methodologies of HiMV for modern multi/many-core CPUs: an H-matrix storage method for efficient memory access, a method that avoids write contentions, an inter-thread load-balancing method, and blocking and sub-matrix sorting methods for cache efficiency.

## [04849] Distributed Graph Neural Network for Billion-Scale Graphs

**Format :** Online Talk on Zoom

**Author(s) :** Israt Nisa (AWS AI)

**Abstract :** GNN models are widely used in recommendation, fraud detection, and search. Real-world graphs from social media and co-purchase networks are large and heterogeneous, posing challenges for scaling training and inference. We demonstrate GraphStorm, a GNN framework that utilizes a distributed hybrid CPU/GPU architecture for efficient graph partitioning, asynchronous computation and data loading, data locality, and hardware utilization (CPU, GPU, network, PCIe).

## [05081] A Framework to Exploit Data Sparsity in Tile Low-Rank Cholesky Factorization

**Format :** Online Talk on Zoom

**Author(s) :** Rabab Mohammad Alomairy (King Abdullah University of Science and Technology)Qinglei Cao (University of Tennessee )Yu Pei (University of Tennessee )george bositca ( University of Tennessee )Hatem Ltaief (King Abdullah University of Science and Technology)David Keyes (King Abdullah University of Science and Technology)Jack Dongarra ( University of Tennessee )

**Abstract :** We accelerate the computations of 3D unstructured mesh deformation based on radial basis function interpolations by exploiting the rank structured property of the matrix. As we increase the accuracy threshold to satisfy the application requirements, the original dense operator gets further compressed and may become sparse enough to switch the dense solver to sparse direct solver. This talk highlights how PaRSEC redistributes the matrix, mitigates the data movement overheads, and copes with the load imbalance.

## [02181] Numerical methods and analysis for linear systems and eigenvalue problems

**Session Time & Room :**

02181 (1/2) : 3C (Aug.23, 13:20-15:00) @E508

02181 (2/2) : 3D (Aug.23, 15:30-17:10) @E508

**Type :** Proposal of Minisymposium

**Abstract :** In this mini-symposium, speakers will present recent developments in the numerical methods for linear systems and eigenvalue problems. The topics of interest include, iterative methods such as IDR(s) and randomized block Kaczmarz methods for linear systems with single right-hand side, and block GMRES-type solvers for linear systems with multiple right-hand sides, acceleration and preconditioning techniques for both linear and nonlinear eigenvalue problems, and algorithms for computing eigenvalues of semi-infinite quasi-Toeplitz matrices.

**Organizer(s) :** Lei Du, Hongjia Chen, Jintao Zhang

**Classification :** 65F10, 65F15

**Minisymposium Program :**

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02181 (1/2) : 3C @E508 [Chair: Hongjia Chen]

## [03254] Interpretation of partial convergence from space partition for linear systems

**Format :** Talk at Waseda University

**Author(s) :** Yanfei Jing (University of Electronic Science and Technology of China)Luc Giraud (Inria Bordeaux -- Sud-Ouest)Yanfei Xiang (Cerfacs, Inria Bordeaux -- Sud-Ouest)

**Abstract :** Efficient solution of large-scale systems of linear equations with multiple right-hand sides is important. Partial convergence and inexact breakdown detection mechanism in the block classical GMRES method characterized by Robbe and Sadkane is a significant progress.

We interpret such partial convergence from space partition, providing flexible choices for approximation search subspace at each iteration.

Beyond, we report our recent progress in block GMRES-type solvers, and show the efficiency of our solvers by some typical numerical experiments..

## [04340] The FEAST algorithm accelerated by subspace expansion for eigenproblems

**Format :** Talk at Waseda University

**Author(s) :** Guojian Yin (Shenzhen University)

**Abstract :** The FEAST algorithm, a contour-integral based eigensolver, was developed for computing the eigenvalues inside a given region, along with their eigenvectors, of generalized eigenproblems. The FEAST algorithm is always fast, stable and easily parallelizable. It can be understood as an accelerated subspace iteration algorithm in conjunction with the Rayleigh–Ritz procedure. Unlike the classic subspace eigensolvers, the FEAST algorithm does not include a subspace expansion procedure when updating the search subspace but filters the search subspace iteratively using an approximate spectral projector. In this talk, I will introduce a subspace expansion scheme for the FEAST algorithm with the hope of producing a better search subspace and the improving convergence rate, especially when it comes to the ill-conditioned problems.

## [03264] Computing eigenvalues of semi-infinite quasi-Toeplitz matrices

**Format :** Talk at Waseda University

**Author(s) :** Dario Bini (University of Pisa) Bruno Iannazzo (University of Perugia) Beatrice Meini (University of Pisa) Jie Meng (Ocean University of China) Leonardo Robol (University of Pisa)

**Abstract :** A quasi-Toeplitz (QT) matrix is a semi-infinite matrix of the form  $A = T(a) + E$  where  $T(a)$  is the Toeplitz matrix with

entries  $(T(a))_{i,j} = a_{j-i}$ , for  $a_{j-i} \in \mathbb{C}$ ,  $i, j \geq 1$ , while  $E$  is a matrix representing a compact operator in  $\ell^2$ . The matrix  $A$  is finitely representable if  $a_k = 0$  for  $k < -m$  and for  $k > n$ , given  $m, n > 0$ , and if  $E$  has a finite number of nonzero entries. The problem of numerically computing eigenpairs of a finitely representable QT matrix is investigated, i.e., pairs  $(\lambda, v)$  such that  $Av = \lambda v$ , with  $\lambda \in \mathbb{C}$ ,  $v = (v_j)_{j \in \mathbb{Z}^+}$ ,  $v \neq 0$ , and  $\sum_{j=1}^{\infty} |v_j|^2 < \infty$ . It is shown that the problem is

reduced to a finite nonlinear eigenvalue problem of the kind  $WU(\lambda)\beta = 0$ , where  $W$  is a constant matrix and  $U$  depends on  $\lambda$  and can be given in terms of either a Vandermonde matrix or a companion matrix.

Algorithms relying on Newton's method applied to the equation  $\det WU(\lambda) = 0$  are analyzed. Numerical experiments show the effectiveness of this approach.

## [03454] Preconditioning techniques for nonlinear eigenvalue problem expressed in non-monomial basis

**Format :** Talk at Waseda University

**Author(s) :** Hongjia Chen (Nanchang University)

**Abstract :** One of the most successful methods for solving a polynomial (PEP) or rational eigenvalue problem (REP) is to recast it, by linearization, as an equivalent but larger generalized eigenvalue problem which can be solved by standard eigensolvers. In this work, we investigate the backward errors of the computed eigenpairs incurred by the application of the well-received compact rational Krylov (CORK) linearization. Our treatment is unified for the PEPs or REPs expressed in various commonly used bases, including Taylor, Newton, Lagrange, orthogonal, and rational basis functions. We construct one-sided factorizations that relate the eigenpairs of the CORK linearization and those of the PEPs or REPs. With these factorizations, we establish upper bounds for the backward error of an approximate eigenpair of the PEPs or REPs relative to the backward error of the corresponding eigenpair of the CORK linearization. These bounds suggest scaling techniques to improve the accuracy of the computed eigenpairs. We show, by numerical experiments, that the actual backward errors can be successfully reduced by scaling and the errors, before and after scaling, are both well predicted by the bounds.

02181 (2/2) : 3D @E508

## [04543] A variant algorithm of the IDR(s) method for solving linear systems

**Format :** Talk at Waseda University

**Author(s) :** Lei Du (Dalian University of Technology)

**Abstract :** The Induced Dimension Reduction method (IDR(s)) proposed by Sonneveld and van Gijzen is an efficient method for solving large, sparse and nonsymmetric linear systems, after then many variants have been proposed. The method has also been generalized to solve matrix equations and eigenvalue problems. In this talk, we consider using the Anderson acceleration technique and propose a new variant to accelerate the IDR(s) method. Some numerical experiments are presented to show the efficiency of our proposed algorithm.

## [03550] Randomized block Kaczmarz methods with k-means clustering for solving linear systems

**Author(s) :** Ke Zhang (Shanghai Maritime University) Xiang-Long Jiang (Shanghai Maritime University) Junfeng Yin (Tongji University)

**Abstract :** In this talk, by following the philosophy of the block Kaczmarz methods, we propose a randomized block Kaczmarz method with the blocks determined by the k-means clustering. It can be considered as an efficient variant of the relaxed greedy randomized Kaczmarz algorithm by using a practical probability criterion for selecting the working block submatrix per iteration. The new algorithm is proved to be convergent when the linear system is consistent. A practical variant of the new method is also given. Some numerical examples are given to verify the effectiveness of the proposed methods.

# [02212] Modeling, Algorithms and Simulations for Flow and Transport in Porous Media

## **Session Time & Room :**

02212 (1/3) : 2C (Aug.22, 13:20-15:00) @D403

02212 (2/3) : 2D (Aug.22, 15:30-17:10) @D403

02212 (3/3) : 2E (Aug.22, 17:40-19:20) @D403

## **Type :** Proposal of Minisymposium

**Abstract :** Porous media flow and transport is important in wide applications, including carbon sequestration, subsurface hydrogen storage, and geothermal reservoirs. This mini-symposium seeks to highlight newest developments of porous media flow and transport both in physical models and numerical methods, to exchange ideas and to promote collaborations. Specific topics of interest include, but are not limited to: advanced physical models of porous media flow and transport; novel numerical methods for its simulation; its machine learning and deep learning algorithms; multiphase and multiphysics simulation; its error estimation, cross-scale analysis, and uncertainty quantification; applications especially in geological carbon sequestration and energy storage.

**Organizer(s) :** Shuyu Sun, James Liu, Ruishu Wang

**Classification :** 76-10, 65M06, 65M08, 65M22

## **Minisymposium Program :**

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02212 (1/3) : 2C @D403

## [03292] Stabilized enhancement for large time computation using exponential spectral process method

### **Author(s) :** Xiang Wang (Jilin University)

**Abstract :** We propose an exponential spectral process (ESP) method for time discretization of spatial-temporal equations. The proposed ESP method uses explicit iterations at each time step, which allows us to use simple initializations at each iteration. This method has the capacity to obtain high accuracy (up to machine precision) with reasonably large time step sizes. Theoretically, the ESP method has been shown to be unconditionally energy stable for arbitrary number of iteration steps for the case where two spectral points are used. To demonstrate the advantages of the ESP approach, we consider two applications that have stability difficulties in large-time simulations. One of them is the Allen-Cahn equation with the symmetry breaking problem that most existing time discretizations face, and the second one is about the complex Ginzburg-Landau equation, which also suffers from large-time instabilities.

## [03294] A pressure robust solver for Stokes flow based on a lifting operator

### **Author(s) :** Ruishu Wang (Jilin University)

**Abstract :** We presents novel finite element solvers for Stokes flow that are pressure-robust due to the use of a lifting operator. Weak Galerkin (WG) finite element schemes are developed for the Stokes problem on quadrilateral and hexahedral meshes. Local Arbogast-Correa or Arbogast-Tao spaces are utilized for construction of discrete weak gradients. The lifting operator lifts WG test functions into  $H(\text{div})$ -subspaces and removes pressure dependence of velocity errors.

## [03331] Numerical Approaches and Analysis for The Generalized Maxwell-Stefan Equations

### **Author(s) :** Xiuping Wang (King Abdullah University of Science and Technology)Shuyu Sun (King Abdullah University of Science and Technology)

**Abstract :** This talk presents an analysis of the thermodynamic properties of the generalized Maxwell-Stefan equations for the diffusion process in multi-component systems and proposes a corresponding numerical scheme. Detailed proofs show that the model satisfies Onsager's principle and the second law of thermodynamics. An energy-stable numerical scheme is established by a mixed finite element method and the backward Euler scheme.

## [03419] The Undrained Split Phase Field Method for Modeling Hydraulic Fracture Propagation

**Author(s)** : Tameem Almani (Saudi Aramco)

**Abstract** : In this work, we present and analyze the undrained split iterative coupling scheme for coupling flow with geomechanics applied to the fracture propagation problem. In the undrained split scheme, the mechanics problem is solved first, followed by the flow problem, and the fluid content of the medium (i.e., porosity) is assumed to be constant during the mechanics solve. This sequential coupling approach was shown to be convergent in an earlier work, and has the advantage of being easier to integrate with legacy reservoir simulators compared to the standard fixed-stress split scheme. This is due to the fact that in the undrained split scheme, the regularization terms are added to the mechanics equation and not the flow equation. In this work, we will establish the convergence of this scheme when applied to the fracture propagation problem using the phase field method. To the best of our knowledge, this is the first time in literature the undrained split scheme is applied to the fracture propagation problem using the phase field method, and the convergence of the combined scheme is established.

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02212 (2/3) : 2D @D403

## [03443] Accelerating Pressure-Temperature Flash Calculations with Physics-informed Neural Networks

**Author(s)** : Yuanqing Wu (Dongguan University of Technology)

**Abstract** : Pressure-Temperature (PT) flash calculations are a performance bottleneck of compositional-flow simulations. With physics-informed neural networks, the two heavy-burden routines of PT flash calculations: the successive substitution technique and stability analysis are avoided in the offline stage, and therefore the computing burden in the offline stage is removed. After training, the phase condition and the compositions can be output by the neural network, which costs much less time than the PT flash calculations.

## [03499] The numerical CFD-DEM model for polymer flooding in weakly consolidated porous media

**Author(s)** : Yerlan Amanbek (Nazarbayev University) Daniyar Kazidenov (Nazarbayev University) Sagyn Omirbekov (Nazarbayev University)

**Abstract** : The study of sand production from the oil and gas reservoirs is an essential for ensuring the long-term viability and profitability of hydrocarbon production operations. In this talk, we present numerical model of polymer flooding using CFD coupled DEM for sand production in 3D. The Navier-Stokes equation is solved using CFD approach, and the DEM approach is based on the second Newton's law to simulate the behavior of individual particles in the porous medium. The modified JKR model is used to represent the weakly consolidated sandstone. The rheology of the injected polymer is described by the power law model. The laboratory experiment was conducted considering the polymer flooding. Numerical model was validated by the sand production rate of the laboratory experiment in the normalized setting.

## [03503] Physics-Preserving Semi-Implicit Schemes for Porous Media Flow with Capillary Heterogeneity

**Author(s)** : Shuyu Sun (KAUST)

**Abstract** : Two-phase flow commonly occurs in environmental engineering and petroleum industry. We present our work on semi-implicit algorithms for two-phase flow in porous media with capillary heterogeneity; in particular, different capillary pressure functions are used for different rock types. Our proposed algorithms, derived from our novel splitting of variables, are locally conservative for both phases, handle capillary heterogeneity well, and are unbiased. The algorithms are also numerically more stable than classical approaches, demonstrated using numerical examples.

## [04169] Efficient numerical methods for thermodynamically consistent model of two-phase flow in porous media

**Author(s)** : Huangxin Chen (Xiamen University)

**Abstract** : In this talk we will introduce a thermodynamically consistent mathematical model for incompressible and immiscible two-phase flow in porous media with rock compressibility. An energy stable numerical method will be introduced, which can preserve multiple physical properties, including the energy dissipation law, full

conservation law for both fluids and pore volumes, and bounds of porosity and saturations. Numerical results are given to verify the features of the proposed methods.

02212 (3/3) : 2E @D403

## **[05155] Geothermal management with an integrated optimization method accelerated by a general thermal decline model and deep learning**

**Author(s)** : Bicheng Yan (King Abdullah University of Science and Technology )Manojkumar Gudala (King Abdullah University of Science and Technology )Shuyu Sun (KAUST)

**Abstract** : Geothermal modeling is complex due to the coupled thermo-hydro-mechanical physics, which brings computational challenges for geothermal management.

To tackle with this, we developed a parsimonious thermal decline model to capture the early thermal breakthrough and the later decline behavior. Further, a forward neural network maps the reservoir parameters to the decline model parameters, and it is integrated with a multi-objective optimizer, which considers reservoir uncertainties and subjects engineering constraints for robust reservoir optimization.

## **[05424] Gym-preCICE: Reinforcement Learning Environments for Active Flow Control**

**Author(s)** : Ahmed H. Elsheikh (Heriot-Watt University)Mosayeb Shams (Heriot-Watt University)

**Abstract** : We introduce Gym-preCICE, a Python adapter to facilitate designing and developing Reinforcement Learning (RL) environments for single- and multi-physics Active flow control (AFC) applications. In an actor-environment setting, Gym-preCICE takes advantage of preCICE, an open-source coupling library for partitioned multi-physics simulations, to handle information exchange between a controller (actor) and an AFC simulation environment. The developed framework results in a seamless non-invasive integration of realistic physics-based simulation toolboxes with RL algorithms.

## **[05495] Ensemble schemes for the numerical solution of a random transient heat equation with uncertain inputs**

**Author(s)** : Xianbing Luo (Guizhou University)Meng Li (Guizhou University)Tingfu Yao (Guizhou University)Changjun Ye (Guizhou University)

**Abstract** : Ensemble-based time stepping schemes are applied to solving a transient heat equation with random Robin boundary and diffusion coefficients. (1) By introducing ensemble mean, we use HDG method to obtain optimal convergence order for random diffusion coefficient problem. (2) By introducing two ensemble means of Robin boundary and diffusion coefficients, we propose a new ensemble Monte Carlo (EMC) scheme for the transient heat equation. (3) By introducing two Max ensemble for Robin boundary and diffusion coefficients problem, we propose a unconditional stability ensemble method. Stability analysis and error estimates are derived. Numerical examples verify the theoretical results and the validity of the ensemble method.

## **[02219] Pattern formation and propagation in reaction-diffusion systems on metric graphs**

**Session Time & Room :**

02219 (1/2) : 3E (Aug.23, 17:40-19:20) @G602

02219 (2/2) : 4C (Aug.24, 13:20-15:00) @G602

**Type** : Proposal of Minisymposium

**Abstract** : This minisymposium concerns theoretical and numerical studies about partial differential equations on metric graphs. Partial differential equations on metric graphs have been applied to a variety of areas as mathematical models related to phenomena in network structures. In particular, this minisymposium focuses on pattern formation and wave propagation in many reaction-diffusion systems on metric graphs, such as Lotka-

part\_2

Volterra systems, Gierer-Meinhardt systems, Allen-Cahn equations, and so on. This minisymposium will invite researchers to report their recent results on these subjects.

**Organizer(s)** : Satoru Iwasaki, Yuta Ishii, Shin-Ichiro Ei, Ken-Ichi Nakamura

**Classification** : 35K57, 35B35, 35B40, 35R02

**Minisymposium Program :**

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02219 (1/2) : 3E @G602 [Chair: Yuta Ishii]

## [05005] Invasion analysis for population dynamics models on simple metric graphs

**Format** : Talk at Waseda University

**Author(s)** : Satoru Iwasaki (Osaka University)Harunori Monobe (Osaka Metropolitan University)

**Abstract** : We are concerned with invasion processes of biological species in network shaped domains, that is metric graphs. In our model, invasions of biological species are restricted by some traps. In this presentation, we report the difference between results of one-dimensional domains case and those of metric graphs case. Particularly, in metric graphs case, we know that vanishing occurs with less traps than one-dimensional case due to an effect of junctions in metric graphs.

## [02969] Propagation phenomena of Fisher-KPP equation in a shifting environment

**Format** : Talk at Waseda University

**Author(s)** : Jong-Shenq Guo (Tamkang University)

**Abstract** : In this talk, we shall discuss the propagation phenomena of the Fisher-KPP equation with a shifting intrinsic growth rate. We divide the heterogeneous shifting term into two different classes, one is the devastating case and the other is the advantageous case. We shall present some results on the existence of forced waves and the spreading dynamics for solutions with compactly supported initial data.

## [03115] Pulse dynamics for reaction-diffusion systems on various metric graphs

**Format** : Talk at Waseda University

**Author(s)** : Shin-Ichiro Ei (Hokkaido University)Haruki Shimatani (Hokkaido University)

**Abstract** : In this talk, we give pulse dynamics for reaction-diffusion systems on various metric graphs. In particular, we analyze the behavior of the pulse solutions by deriving an equation of the motion. Note an equation of the motion is an expression for the time evolution of the positions of pulse solutions. In the same way, we will also discuss front dynamics for reaction-diffusion systems on various metric graphs.

## [03288] Reaction-advection-diffusion equations over simple graphs

**Format** : Talk at Waseda University

**Author(s)** : Bendong Lou (Shanghai Normal University)

**Abstract** : I will talk about the dynamical behavior of a species spreading in a river network, which is modeled by advective diffusion equations over simple graphs with Fisher-KPP or bistable reactions. Denote by  $c_*$  the (minimal) speed of the traveling waves of the corresponding equations without advections, I will present the long time behavior for the solutions in the special case where the water flow speed in upstream is larger than  $c_*$  and that in downstream is smaller than  $c_*$ , which includes washing out, persistence at carrying capacity or persistence below carrying capacity. (joint works with Y. Du, R. Peng, M. Zhou, Y. Morita).

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02219 (2/2) : 4C @G602 [Chair: Satoru Iwasaki]

## [04149] The effect of advection on spike solutions for the Schnakenberg model on Y-shaped metric graph

**Format :** Talk at Waseda University

**Author(s) :** Yuta Ishii (National Institute of Technology, Ibaraki College)

**Abstract :** In this talk, we consider one-peak solutions for the Schnakenberg model with advection term on Y-shaped metric graph. The location and amplitude of the spike are decided by the interaction of the advection with the geometry of Y-shaped graph. In particular, the effect of the advection on the location of the spike depends on the choice of boundary conditions strongly.

## [03837] Turing instability and bifurcation in reaction-diffusion systems on metric graphs

**Format :** Talk at Waseda University

**Author(s) :** Junping Shi (College of William & Mary)

**Abstract :** We show that under a general framework, a constant equilibrium in a time-evolution system could lose its stability with the addition of distinct dispersal rates for different species. Spontaneous symmetry breaking bifurcations occur so non-constant stationary patterns emerge. This is the classical Turing instability and bifurcations. We will show the application of this general scenario to the case of (i) an ODE system on a weighted directed graph, and (ii) a reaction-diffusion system on a metric graph.

## [04417] Front propagation for Lotka-Volterra competition-diffusion system on unbounded star graphs

**Format :** Talk at Waseda University

**Author(s) :** Ken-Ichi Nakamura (Meiji University)

**Abstract :** We consider the 2-component Lotka-Volterra competition-diffusion system in an infinite star graph with a single junction. Under strong competition conditions, we give sufficient conditions for the success/failure of the invasion of superior species beyond the junction. The method is based on a standard argument by constructing super-subsolutions with the help of a new result on the speed of traveling waves for the Lotka-Volterra competition-diffusion system on the whole line.

# [02221] Recent progress on mathematical theory of boundary layer

**Session Time & Room :**

02221 (1/2) : 2E (Aug.22, 17:40-19:20) @G802

02221 (2/2) : 3C (Aug.23, 13:20-15:00) @G802

**Type :** Proposal of Minisymposium

**Abstract :** Boundary effect and stability analysis in fluid mechanics involves many mathematical problems, including boundary layer, free boundary, stability and instability of the hydrodynamic equations under the high Reynolds number, etc. The research on these problems is not only mathematically important and challenging, but also provides specific views for explaining certain physical phenomena and mechanical laws. In order to enhance the exchange on the latest research results and facilitate the cooperations on hydrodynamic stability theory, we would like to organize a mini-symposium named "Recent progress on mathematical theory of boundary layer".

**Organizer(s) :** Zhifei Zhang, Guilong Gui, Yong Lu, Chao Wang

**Classification :** 35QXX, 76FXX, 35FXX

**Minisymposium Program :**

02221 (1/2) : 2E @G802 [Chair: Zhifei Zhang]

## [03046] Eckhaus instability of the compressible Taylor vortex

**Format :** Talk at Waseda University

**Author(s) :** Yoshiyuki Kagei (Tokyo Institute of Technology)

**Abstract :** This talk is concerned with the bifurcation and stability of the compressible Taylor vortex. It is shown that Taylor vortices bifurcate near the criticality for the incompressible problem when the Mach number is sufficiently small. The localized stability of the compressible Taylor vortices is considered and it is shown that the Eckhaus instability of compressible Taylor vortices occurs as in the case of the incompressible ones.

## [03064] Stability of shear flows in inviscid and viscous fluids

**Format :** Talk at Waseda University

**Author(s) :** Weiren Zhao (New York University Abu Dhabi)

**Abstract :** In this talk, I will present some recent progress in the asymptotic stability of shear flows in both inviscid and viscous fluids. The inviscid damping and enhanced dissipation phenomenon will be discussed in both linear and nonlinear models.

## [03247] Tollmien-Schlichting waves in the subsonic regime

**Format :** Talk at Waseda University

**Author(s) :** Di Wu (South China University of Technology)Nader Masmoudi (New York University Abu Dhabi)Yuxi Wang (Sichuan University)Zhifei Zhang (Peking University)

**Abstract :** The Tollmien-Schlichting (T-S) waves play a key role during the early stage of the boundary layer transition. In a breakthrough work, Grenier, Guo and Nguyen gave a first rigorous construction of the T-S waves of temporal mode for the incompressible fluid. In this paper, we construct the T-S waves of both temporal mode and spatial mode to the linearized compressible Navier-Stokes system around the boundary layer flow in the whole subsonic regime. The proof is based on a new iteration scheme via solving two quasi-compressible systems related to the incompressible part and compressible part respectively. For the incompressible part, the key ingredient is to solve an Orr-Sommerfeld type equation, which is based on a new Airy-Airy-Rayleigh iteration instead of Rayleigh-Airy iteration introduced by Grenier, Guo and Nguyen.

## [04253] Global Existence of Weak Solutions for Compressible Navier--Stokes--Fourier Equations with the Truncated Virial Pressure Law

**Format :** Talk at Waseda University

**Author(s) :** Fei Wang (Shanghai Jiao Tong University)Didier Bresch (Univ. Savoie Mont Blanc)Pierre-Emmanuel Jabin (Pennsylvania State University)

**Abstract :** This paper concerns the existence of global weak solutions {it 'a la Leray} for compressible Navier-Stokes--Fourier system with periodic boundary conditions and the truncated virial pressure law which is assumed to be thermodynamically unstable. More precisely, the main novelty is that the pressure law is not assumed to be monotone with respect to the density. This provides the first global weak solutions result for the compressible Navier-Stokes-Fourier system with such kind of pressure law which is strongly used as a generalization of the perfect gas law. The paper is based on a new construction of approximate solutions through an iterative scheme and fixed point procedure which could be very helpful to design efficient numerical schemes. Note that our method involves the recent paper by the authors published in Nonlinearity (2021) for the compactness of the density when the temperature is given.

02221 (2/2) : 3C @G802 [Chair: Guiding Gui]

## [03513] Nonlinear Stability of the Taylor-Couette flow

**Format :** Talk at Waseda University

**Author(s) :** Te Li (National University of Singapore)

**Abstract :** Hydrodynamic stability at high Reynolds number is a central topic in fluid mechanics. It is closely related to turbulence. Whereas the laminar velocity profile is linearly stable for all Reynolds number, Reynolds experiment reveals that laminar flows could be unstable and transit to turbulence at high Reynolds number. This phenomenon is described as subcritical transition. And the mechanism behind is not well understood yet. To investigate the dynamical nonlinear stability, we develop a systematic approach to establish sharp resolvent estimates for the linearized operator around the 2D Taylor-Couette flow. One of the main difficulties is that the linearized operator is non-self-adjoint. Based on the resolvent estimates, we first show the sharp enhanced-dissipation decay rate of the solution for the linearized system. We also derive the space-time estimates for the

nonlinear part using the resolvent estimates. Combining all above, we obtain the nonlinear transition threshold for the Taylor-Couette flow. This talk is based on a series of joint works by X. An-T. He-L.

## [04401] On the solvability of the linearized Triple-Deck system

**Format :** Online Talk on Zoom

**Author(s) :** Yasunori Maekawa (Kyoto University)David Gerard-Varet (Universite Paris Cite et IMJ-PRG)Sameer Iyer (University of California)

**Abstract :** We establish the solvability of the linearized Triple-Deck system in Gevrey 3/2 regularity in the tangential variable, under the concavity assumptions on the background flow. This talk is based on the joint work with David Gerard-Varet (Universite Paris Cite et IMJ-PRG) and Sameer Iyer (University of California).

## [03016] On dynamic stability for steady Prandtl solutions

**Format :** Online Talk on Zoom

**Author(s) :** Yue Wang (Capital Normal University)

**Abstract :** In this talk, I will first review some properties of steady Prandtl solutions. Then I will introduce our recent work on dynamic stability of steady Prandtl solutions( a joint work with Yan Guo and Zhifei Zhang) and others' related results.

# [02277] New regularizing algorithms for solving inverse and ill-posed problems

**Session Time & Room :**

02277 (1/6) : 3E (Aug.23, 17:40-19:20) @G809

02277 (2/6) : 4C (Aug.24, 13:20-15:00) @G809

02277 (3/6) : 4D (Aug.24, 15:30-17:10) @G809

02277 (4/6) : 4E (Aug.24, 17:40-19:20) @G809

02277 (5/6) : 5B (Aug.25, 10:40-12:20) @G809

02277 (6/6) : 5C (Aug.25, 13:20-15:00) @G809

**Type :** Proposal of Minisymposium

**Abstract :** Regularization methods are an important numerical technique in the robust solution of ill-posed inverse problems. In the recent years, many new regularization methods had been developed in various areas of applied mathematics and data science. This minisymposium focuses on the regularization theory of abstract (linear and nonlinear) operator equations and some efficient regularizing algorithms for solving parameter identification problems in (local and nonlocal) PDEs. Such regularizing algorithms includes stochastic asymptotic regularization for general operator equation, asymptotic expansion regularization for inverse problems in singularly perturbed PDEs, machine learning based approaches, etc. The speakers mainly from Russia and China.

**Organizer(s) :** Ye Zhang, Maxim Shishlenin, Anatoly Yagola and Sergey Kabanikhin

**Classification :** 35R30, 47A52, 65R30, 65N30, 35N25

**Minisymposium Program :**

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02277 (1/6) : 3E @G809

## [05628] Regularization of linear inverse problems and neural networks

**Format :** Online Talk on Zoom

**Author(s) :** Sergey Kabanikhin (Sobolev Institute of Mathematics)

**Abstract :** The report will consider methods of numerical regularization of linear inverse problems and neural networks in applications.

## [05627] Applied inverse problems for parabolic equations

**Format :** Online Talk on Zoom

**Author(s) :** Maxim Shishlenin (Sobolev Institute of Mathematics)

**Abstract :** The report will consider inverse problems for parabolic equations in applications such as pharmacodynamics and financial mathematics.

## [02806] Data-Driven Regularization in Variational Data Assimilation from An Ocean Perspective

**Format :** Talk at Waseda University

**Author(s) :** Long Li (Harbin Institute of Technology) Jianwei Ma (Peking University)

**Abstract :** Current machine learning-driven methods make a positive difference to outlook on data assimilation. However, its reliability remains to be studied since little deterministic information from physical laws is involved. In this talk, we will introduce our recent work about the efficient assimilation by the approximation of a deep neural network. The sparsity regularization is employed to improve the well-posedness. Results show the technique is robust for reconstructing the velocity of a fluid with vortex structures.

## [02803] Uniqueness and numerical inversion in the time-domain fluorescence diffuse optical tomography

**Format :** Talk at Waseda University

**Author(s) :** Chunlong Sun (Nanjing University of Aeronautics and Astronautics)

**Abstract :** This work considers the time-domain fluorescence diffuse optical tomography. We recover the distribution of fluorophores in biological tissue by the boundary measurements. With the Laplace transform and the knowledge of complex analysis, we build the uniqueness theorem of this inverse problem. The numerical inversions are considered. We introduce an iterative inversion algorithm under the framework of regularizing scheme.

02277 (2/6) : 4C @G809

## [02839] Stochastic asymptotical regularization for nonlinear ill-posed problems

**Format :** Talk at Waseda University

**Author(s) :** Haie Long (Shenzhen SMU-BIT University)

**Abstract :** In this paper, we establish an initial theory regarding the stochastic asymptotical regularization (SAR) for the uncertainty quantification of the stable approximate solution of ill-posed nonlinear-operator equations, which are deterministic models for numerous inverse problems in science and engineering. By combining techniques from classical regularization theory and stochastic analysis, we prove the regularizing properties of SAR with regard to mean-square convergence. The convergence rate results under the canonical sourcewise condition are also studied. Several numerical examples are used to show the accuracy and advantages of SAR: compared with the conventional deterministic regularization approaches for deterministic inverse problems, SAR can provide the uncertainty quantification of a solution and escape local minimums for nonlinear problems.

## [03062] A new framework to quantify the uncertainty in inverse problems

**Format :** Talk at Waseda University

**Author(s) :** Wenlong Zhang (Southern University of Science and Technology)

**Abstract :** In this work, we investigate the regularized solutions and their finite element solutions to the inverse problems governed by partial differential equations, and establish the stochastic convergence and optimal finite element convergence rates of these solutions, under point wise measurement data with random noise. The regularization error estimates and the finite element error estimates are derived with explicit dependence on the noise level, regularization parameter, mesh size, and time step size, which can guide practical choices among these key parameters in real applications. The error estimates also suggest an iterative algorithm for determining an optimal regularization parameter.

## [03104] Numerical algorithms for solving the nonlinear Schrödinger equation

**Format :** Talk at Waseda University

**Author(s) :** Shuang Liu (Novosibirsk State University)

**Abstract :** In this paper, the Physical Information Neural Networks algorithm is used to solve the nonlinear Schrödinger equation in a dispersed medium. Adaptive activation functions are used to accelerate PINN convergence, and this approach uses very little data to obtain an exact solution. Due to the approximation capability of the neural network, the results are used in semiconductor optical amplifier fiber lasers where nonlinear effects allow spectral tuning of the generated pulses.

## [03354] Multidimensional Ill-Posed Problems in Applications

**Format :** Talk at Waseda University

**Author(s) :** Anatoly Yagola (Lomonosov Moscow State University)

**Abstract :** The report will consider applied multidimensional inverse problems of geophysics (magnetometry and gravimetry) and electron microscopy (electron backscattering), regularizing algorithms for their solution and the results of experimental data processing.

02277 (3/6) : 4D @G809

## [04375] Solution of inverse problems in three-dimensional singularly perturbed PDEs

**Format :** Talk at Waseda University

**Author(s) :** Dmitrii Chaikovskii (Shenzhen MSU-BIT University)Ye Zhang (Beijing Institute of Technology)

**Abstract :** We present an efficient asymptotic expansion method for solving forward and inverse problems in a nonlinear, time-dependent, singularly perturbed reaction-diffusion-advection equation. We prove the existence and uniqueness of a smooth solution in 3D PDEs using asymptotic expansion. A simplified equation for the inverse source problem is derived, maintaining accuracy even with noisy data. We propose an asymptotic expansion regularization algorithm for the 3D inverse source problem and demonstrate its feasibility through a model problem.

## [05101] The coupled complex boundary methods for inverse problems of partial differential equations

**Format :** Talk at Waseda University

**Author(s) :** Rongfang Gong (Nanjing University of Aeronautics and Astronautics)

**Abstract :** In this talk, a coupled complex boundary method (CCBM) is proposed for an inverse source problem. With the introduction of imaginary unit, the CCBM transfers the original real problem to a complex one. The CCBM has several merits and is further improved. Also, the applications of the CCBM to bioluminescence tomography, inverse Cauchy problem, chromatography etc. are delivered.

## [05498] Physics-informed invertible neural network for the Koopman operator learning

**Format :** Talk at Waseda University

**Author(s) :** Yue Qiu (Chongqing University)

**Abstract :** The Koopman operator is used to embed a nonlinear system into an infinite, yet linear system with a set of observable functions. However, manually selecting observable functions that span the invariant subspace of the Koopman operator based on prior knowledge is inefficient and challenging, particularly when little or no information is available about the underlying systems. Furthermore, current methodologies tend to disregard the importance of the invertibility of observable functions, which leads to inaccurate results. To address these challenges, we propose the so-called FlowDMD, a Flow-based Dynamic Mode Decomposition that utilizes the Coupling Flow Invertible Neural Network (CF-INN) framework. FlowDMD leverages the intrinsically invertible characteristics of the CF-INN to learn the invariant subspaces of the Koopman operator and accurately reconstruct state variables. Numerical experiments demonstrate the superior performance of our algorithm compared to state-of-the-art methodologies.

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02277 (4/6) : 4E @G809

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02277 (5/6) : 5B @G809

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02277 (6/6) : 5C @G809

## [02285] New Trends in Tensor Networks and Tensor Optimization

**Session Time & Room :**

02285 (1/2) : 4D (Aug.24, 15:30-17:10) @A208

02285 (2/2) : 4E (Aug.24, 17:40-19:20) @A208

**Type :** Proposal of Minisymposium

**Abstract :** Tensors have been shown to be a powerful tool for capturing multiple interactions and inherent hierarchies in data sets from wide applications in scientific and engineering communities. This minisymposium aims to bring together recent advances in tensor network analysis and large-scale tensor optimization. The topics of interest include, but are not limited to

- new advances in tensor networks for machine learning,
- tensorial time series analysis and deep learning,
- tensor regularized generalization in reinforcement learning,
- structural tensor analysis and applications,
- multilinear PageRank and data clustering.

**Organizer(s) :** Qibin Zhao, Yannan Chen, Andong Wang

**Classification :** 90C90

**Minisymposium Program :**

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02285 (1/2) : 4D @A208

## [03267] Efficient Machine Learning with Tensor Networks

**Format :** Online Talk on Zoom

**Author(s) :** Qibin Zhao (RIKEN AIP)

**Abstract :** Tensor Networks (TNs) are factorizations of high dimensional tensors into networks of many low-dimensional tensors, which have been studied in quantum physics, high-performance computing, and applied mathematics. In recent years, TNs have been increasingly investigated and applied to machine learning and signal processing, due to its significant advances in handling large-scale and high-dimensional problems, model compression in deep neural networks, and efficient computations for learning algorithms. This talk aims to present some recent progress of TNs technology applied to machine learning from perspectives of basic principle and algorithms, novel approaches in unsupervised learning, tensor completion, multi-model learning and various applications in DNN, CNN, RNN and etc.

## [05506] Accelerated Doubly Stochastic Gradient Descent for Tensor CP Decomposition

**Format :** Talk at Waseda University

**Author(s) :** Chunfeng Cui (Beihang University)

**Abstract :** In this talk, we focus on the doubly stochastic gradient descent (SGD) method for computing the canonical polyadic decomposition (CPD) of tensors. This method not only exploits the block structure of CPD but also enables us to handle large-scale tensors. Based on the momentum acceleration and the variance reduction technique, we propose several acceleration methods, including the heavy-ball acceleration, inertial acceleration, and variance reduction. We also present the global convergence and convergence rates of the proposed methods.

## [03184] Tensor network strcuture search

**Format :** Talk at Waseda University

**Author(s) :** Chao Li (RIKEN)

**Abstract :** In this talk, we present a novel problem related to model selection for tensor networks, which we call tensor network structure search (TN-SS). TN-SS aims to find the optimal tensor network structure for a given dataset and task by exploring a large space of possible network structures. We propose several promising solutions to the TN-SS problem, including evolutionary algorithms, stochastic search, and alternating enumeration. Our methods are designed to efficiently explore the space of tensor network structures and identify the most promising candidates based on their performance on the given task.

## [04779] Towards Multi-modes Outlier Robust Tensor Ring Decomposition

**Format :** Talk at Waseda University

**Author(s) :** Yuning Qiu (Guangdong University of Technolog)

**Abstract :** The outliers assumption in conventional robust tensor decomposition is often not true in tensors since high-order tensors are prone to be corrupted by outliers in more than one direction. To mitigate this weakness, we propose a novel outlier robust tensor decomposition (ORTD) model by capturing low-rank tensors corrupted from multi-mode outliers. To theoretically guarantee statistical performance, we rigorously analyze a non-asymptotic upper bound of the estimation error for the proposed ORTD model.

02285 (2/2) : 4E @A208

## [05508] Singular Value Decomposition of Dual Matrices and its Application to Traveling Wave Identification in the Brain

**Format :** Talk at Waseda University

**Author(s) :** Tong Wei (Fudan University)Weiyang Ding (Fudan University)Yimin Wei (Fudan University)

**Abstract :** atrix factorization in dual number algebra, a hypercomplex system, has been applied to kinematics, mechanisms, and other fields recently. We develop an approach to identify spatiotemporal patterns in the brain such as traveling waves using the singular value decomposition of dual matrices. Theoretically, we propose the compact dual singular value decomposition (CDSVD) of dual complex matrices with explicit expressions as well as a necessary and sufficient condition for its existence. Furthermore, based on the CDSVD, we report on the optimal solution to the best rank-k approximation under a newly defined quasi-metric in dual complex number system. The CDSVD is also related to the dual Moore-Penrose generalized inverse. Numerically, comparisons with other available algorithms are conducted, which indicate the less computational cost of our proposed CDSVD. Next, we employ experiments on simulated time-series data and a road monitoring video to demonstrate the beneficial effect of infinitesimal parts of dual matrices in spatiotemporal pattern identification. Finally, we apply this approach to the large-scale brain fMRI data and then identify three kinds of traveling waves, and further validate the consistency between our analytical results and the current knowledge of cerebral cortex function.

## [03043] Multilinear Pseudo-PageRank for Hypergraph Partitioning

**Format :** Talk at Waseda University

**Author(s) :** Yannan Chen (South China Normal University)

**Abstract :** In this talk, we establish the higher-order pseudo-PageRank model, which is formulated as a multilinear system with nonnegative constraints. The coefficient tensor of the multilinear system is a kind of Laplacian tensor of the uniform hypergraph and no dangling corrections are involved. Then, a tensor splitting algorithm is utilized for solving the higher-order pseudo-PageRank problem, of which solutions exist but may not be unique. Numerical experiments illustrate that the proposed higher-order pseudo-PageRank method is powerful and effective for hypergraph partitioning problems.

## [04276] Tensorial Time Series Prediction via Tensor Neural Differential Equations

**Format :** Talk at Waseda University

**Author(s) :** Mingyuan Bai (RIKEN AIP)

**Abstract :** The recent decade has witnessed the surge of models and applications in multi-dimensional, i.e., tensorial time series analysis, where their entanglement of different aspects of data, i.e., modes, appeals to both academia and industry, and raises a number of challenges for modeling and analysis. To address these challenges,

we aim to introduce tensor neural differential equations for tensorial time series analysis, including tensor neural ordinary differential equations and tensor neural controlled differential equations, etc.

## [03838] A gradient projection method for semi-supervised hypergraph clustering problems

**Format :** Talk at Waseda University

**Author(s) :** Jingya Chang (Guangdong University of Technology)

**Abstract :** We use the hypergraph related tensor to construct an orthogonal constrained optimization model for the semi-supervised hypergraph problems, which is solved by a retraction method. A nonmonotone curvilinear search is implemented to guarantee reduction in the objective function value. Experiments on synthetic hypergraph and hypergraph given by real data demonstrate the effectivity of our method.

## [02327] Stability of Numerical Linear Algebra Algorithms

**Session Time & Room :**

02327 (1/2) : 3E (Aug.23, 17:40-19:20) @E508

02327 (2/2) : 4C (Aug.24, 13:20-15:00) @E508

**Type :** Proposal of Minisymposium

**Abstract :** The stability of numerical linear algebra algorithms is a key component in large-scale and delicate computations such as solutions of linear systems of equations, eigenvalue problems, and matrix function computations. These computations in common require efficient but stable orthogonalization techniques. Understanding their numerical behaviors is thus equally important as their parallel efficiency. Recent low-synchronization and mixed-precision algorithms do improve parallel scaling while maintaining numerical stability when using next-generation high-performance computers. This minisymposium will foster interactions between new results of error analyses and new algorithmic innovations, and so will contribute to communication inside and beyond these two communities.

**Organizer(s) :** Keiichi Morikuni, Miroslav Rozložník

**Classification :** 65F10, 65F25, 65F60, 65F35, 65Y05

**Minisymposium Program :**

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02327 (1/2) : 3E @E508 [Chair: Keiichi Morikuni]

## [02923] A projection method for singular eigenvalue problems of linear matrix pencils

**Format :** Talk at Waseda University

**Author(s) :** Keiichi Morikuni (University of Tsukuba)Akira Imakura (University of Tsukuba)

**Abstract :** Complex moments consisting of matrix resolvents filter out undesired eigencomponents and extract the desired ones from a pseudo-random matrix. This study extends a projection method using complex moments for regular eigenproblems to the singular nonsquare case. We establish conditions such that the method gives all finite eigenvalues in a prescribed region in the complex plane and the corresponding eigenvectors. Numerical experiments show that the new method is more robust and efficient than previous methods.

## [03257] Backward stability in rational eigenvalue problems solved via linearization

**Format :** Talk at Waseda University

**Author(s) :** Froilán Martínez Dopico (Universidad Carlos III de Madrid)María del Carmen Quintana (Aalto University )Paul Van Dooren (Université catholique de Louvain)

**Abstract :** The numerical solution of nonlinear eigenvalue problems has attracted a lot of attention from the Numerical Linear Algebra community in the last twenty years. Among these problems, rational eigenvalue problems are particularly relevant because they appear directly in many applications and because they are often used to approximate other more general nonlinear eigenvalue problems. One of the most reliable methods for

solving numerically rational eigenvalue problems is via linearizations. In this talk we present recent results on the backward stability of this approach.

## [03008] Computing the matrix sign function with the double exponential formula

**Format :** Talk at Waseda University

**Author(s) :** Tomoya Miyashita (The University of Electro-Communications)Shuhei Kudo (The University of Electro-Communications)Yusaku Yamamoto (The University of Electro-Communications)

**Abstract :** Matrix sign function plays an important role in many scientific computations. There are various methods for computing the matrix sign function, such as Newton's method, the Schur method, and methods based on integral representation. Among them, the integral-based methods are suitable for parallelization because the calculation at each sample point is independent. In this talk, we focus on the integral-based method using the double exponential (DE) formula recently proposed by Nakaya and Tanaka and evaluate its numerical accuracy and parallel performance on the Fugaku computer. We also show a new theoretical upper bound on its discretization and truncation errors.

## [03899] Mixed Precision Strategies for Preconditioned Restarted GMRES

**Format :** Online Talk on Zoom

**Author(s) :** Theo Mary (Sorbonne Université, CNRS, LIP6)Alfredo Buttari (Université de Toulouse, CNRS, IRIT)Nicholas J Higham (The University of Manchester)Bastien Vieublé (The University of Manchester)

**Abstract :** The GMRES method, along with its flexible variants, is one of the most popular algorithms to solve large sparse linear systems. In its 40-year history, many different mixed precision strategies for GMRES have been proposed. Yet, there is no consensus on which of these strategies works best, nor even a good understanding of their numerical behavior.

The goal of this work is to develop a systematic error analysis of (preconditioned, restarted, possibly flexible) GMRES in a framework as generic as possible, that encompasses existing strategies and reveals new opportunities.

02327 (2/2) : 4C @E508 [Chair: Miroslav Rozložník]

## [04236] Numerical stability of block classical Gram-Schmidt process

**Format :** Talk at Waseda University

**Author(s) :** Miroslav Rozložník (Czech Academy of Sciences)Erin Claire Carson (Charles University)Kathryn Lund (Charles University)

**Abstract :** The block version of the classical Gram-Schmidt (BCGS) method is often employed to efficiently compute orthogonal bases for Krylov subspace methods and eigenvalue solvers, but a rigorous proof of its stability behavior has not yet been established. It is shown that the usual implementation of BCGS can lose orthogonality at a rate worse than  $O(\varepsilon)\kappa^2(X)$ , where  $X$  is the input matrix and  $\varepsilon$  is the unit roundoff. A useful intermediate quantity denoted as the Cholesky residual is given special attention and, along with a block generalization of the Pythagorean theorem, this quantity is used to develop more stable variants of BCGS. These variants are proven to have at most  $O(\varepsilon)\kappa^2(X)$  loss of orthogonality with relatively relaxed conditions on the intrablock orthogonalization routine satisfied by the most commonly used algorithms. A variety of numerical examples illustrate the theoretical bounds.

## [02742] Cross-interactive residual smoothing for block Lanczos-type methods for solving linear systems with multiple right-hand sides

**Format :** Talk at Waseda University

**Author(s) :** Kensuke Aihara (Tokyo City University)Akira Imakura (University of Tsukuba)Keiichi Morikuni (University of Tsukuba)

**Abstract :** Block Lanczos-type methods often exhibit large oscillations in the residual norms, leading to a large residual gap and a loss of attainable accuracy of the approximations. Cross-interactive residual smoothing (CIRS) was recently developed for the standard/global Lanczos-type methods to obtain smooth convergence behavior and reduce the residual gap. We therefore extend CIRS to the block version. Rounding error analysis and numerical experiments demonstrate the effectiveness of the presented approach.

## [02706] Gauss-Seidel (MGS) - Jacobi (CGS) GMRES with Rank-1 Perturbation Smoothers

**Format :** Online Talk on Zoom

**Author(s) :** Stephen Thomas (Advanced Micro Devices) Miro Rozloznik (Czech Academy of Science) Erin Carson (Charles University)

**Abstract :** We introduce a low-synch GMRES algorithm based on Gauss-Seidel (MGS) and Jacobi (CGS) iterations. The correction matrix  $T = (I + L)^{-1}$  for the projector  $P = I - QTQ^T$  is a rank-1 perturbation, and results in low backward error. These ideas are applied to AMG. The smoother performs a triangular solve and subsequent iterations apply Jacobi or  $(I - uv^T)r_k$ ,  $u = L_{k,1:k-1}$  and  $v = e_k$ . GMRES convergence remains the same with this iterative refinement.

## [05049] Improving convergence and stability of Krylov subspace methods for solving linear systems

**Format :** Talk at Waseda University

**Author(s) :** hassane sadok (université du Littoral Cote d'Opale)

**Abstract :** Krylov subspace methods are widely used for the iterative solution of a large variety of linear systems of equations with one or several right hand sides or for solving nonsymmetric eigenvalue problems. The purpose of this talk is to compare several variants of the implementation of Krylov subspace methods, including GMRES, QMR, and CMRH methods. These schemes are based on the two-sided Gram-Schmidt process methods and differ in their use of the inner product (=) where ( $P = I - C C^+$ ) is a projector. We provide a unified description of the methods discussed and derive new expressions and bounds for the residual errors.

## [02342] On dataset sparsification and data reconstruction in deep learning

**Session Time & Room :** 3D (Aug.23, 15:30-17:10) @E817

**Type :** Proposal of Minisymposium

**Abstract :** Recent successes in deep learning are partially driven by the ability to use ever larger datasets with overparametrized models. However, the ability to obtain similar performance over smaller datasets is clearly computationally advantageous. Furthermore, when learning with large models over large datasets, it has been shown that portions of the data can be reconstructed from the model parameters. This clearly poses a privacy risk. It turns out that dataset reconstruction and dataset distillation are closely related. This symposium will bring together researchers working on the latest advances in both dataset reconstruction and distillation.

**Organizer(s) :** Anastasia Borovykh

**Classification :** 68T07, 90C31

**Minisymposium Program :**

02342 (1/1) : 3D @E817 [Chair: Anastasia Borovykh]

## [03191] Data sampling for surrogate modeling and optimization

**Format :** Talk at Waseda University

**Author(s) :** Tyler H Chang (Argonne National Laboratory)

**Abstract :** In surrogate modeling for nonconvex blackbox optimization, global convergence is driven by the global approximation error of an interpolatory model. For large complex problems, achieving global model accuracy can be prohibitively expensive, so model-based optimization techniques such as Bayesian optimization rely on adaptive sampling to tradeoff between exploration and exploitation. However, these techniques are known to scale poorly with dimension. Therefore, we analyze an alternative approach based on response surface methodology coupled with static design-of-experiments.

## [03317] Bayesian inference via dataset sparsification

**Format :** Online Talk on Zoom

**Author(s) :** Trevor Campbell (UBC)

**Abstract :** A Bayesian coresnet is a sparsified dataset that can be used to reduce the cost of inference. Constructing high-quality coresnets remains a challenge. In this work we introduce a new method for coresnet construction that involves subsampling the data, and then optimizing a variational flow parametrized by coresnet weights. Theoretical results demonstrate that our method achieves exponential data compression in a representative model. Experiments demonstrate accurate inference with reduced runtime compared with standard inference methods.

## [03934] Foundations of Information Leakage in Machine Learning

**Format :** Talk at Waseda University

**Author(s) :** Reza Shokri (National University of Singapore)

**Abstract :** This talk will explore the foundations of data privacy in machine learning, with a specific focus on membership inference attacks.

## [04492] Understanding Reconstruction Attacks with Dataset Distillation

**Format :** Talk at Waseda University

**Author(s) :** Noel Loo (Massachusetts Institute of Technology)

**Abstract :** Dataset reconstruction attacks are attacks which aim to recover portions of training data from a trained neural network with access to only the model parameters. In this talk, we study the efficacy of these attacks in both infinite and finite-width regimes, and show that these reconstruction attacks are closely related to dataset distillation. In doing so, we study the properties of recovered images, namely what makes images easy to reconstruct, and how they affect training.

# [02349] Deep Implicit and Explicit Models for Inverse Problems: Hybrid Data-Driven Models, Neural ODEs, PDEs and Beyond

**Session Time & Room :**

02349 (1/3) : 3E (Aug.23, 17:40-19:20) @E817

02349 (2/3) : 4C (Aug.24, 13:20-15:00) @E817

02349 (3/3) : 4D (Aug.24, 15:30-17:10) @E817

**Type :** Proposal of Minisymposium

**Abstract :** In this minisymposium, we will discuss the current developments of implicit and explicit deep learning models for inverse problems. Explicit deep learning models are based on stacking several discrete layers to solve a given downstream tasks. Another interesting perspective is implicit models, where one can specify the conditions to satisfy. Within this context our session will cover these two paradigms through new developments in Hybrid Models, Neural ODES – PDEs and Beyond. Moreover, discussing interesting real-world applications for a wide range of inverse problems.

**Organizer(s) :** Angelica Aviles-Rivero, Raymond H. Chan

**Classification :** 68T07, 65K10, 49N45

**Minisymposium Program :**

02349 (1/3) : 3E @E817

## [05633] Why Deep Surgical Models Fail?: Revisiting Surgical Action Triplet Recognition through the Lens of Robustness

**Author(s)** : Yanqi Cheng (University of Cambridge )

**Abstract** : Surgical action triplet recognition is of high relevance as it provides the surgeon with context-aware support and safety. The go-to strategy develops new network mechanisms. However, the performance of state-of-the-art techniques is substantially lower than other surgical tasks. Why is this happening? This is the question that we address in this work. We present the first study to understand the failure of existing deep learning models through the lens of robustness and explainability.

## [05634] On Implicit Neural Representation

**Author(s)** : Zhenda Shen (City University of Hong Kong)

**Abstract** : In this talk, we explore a novel approach to implicit neural representations, introducing a novel function that capitalizes on the advantages of Strong Spatial and Frequency attributes. Unlike conventional methods, our proposed technique exhibits remarkable performance improvements across a diverse range of downstream tasks. Through rigorous experimentation and validation, we demonstrate the superior capabilities of our new function in critical applications such as denoising, CT reconstruction, and 3D reconstruction.

Implicit neural representations have garnered significant interest in recent years due to their ability to model complex and high-dimensional data without requiring explicit parameterization. Our novel function leverages both spatial and frequency domains, enhancing its ability to capture intricate patterns and relationships within the data.

During the presentation, we delve into the technical details of our approach, providing insights into how we use spatial and frequency information effectively. We highlight the advantages of our technique over existing methods, emphasizing the superior performance and efficiency it offers.

Through extensive experimental evaluations, we showcase how our new function excels in denoising tasks, enabling high-fidelity reconstructions even in noisy environments. Additionally, we demonstrate its exceptional capabilities in CT reconstruction, where our approach delivers accurate and robust results with reduced artifacts. Furthermore, in the realm of 3D reconstruction, our method outperforms existing techniques, offering more precise and detailed representations.

02349 (2/3) : 4C @E817 [Chair: Raymond H Chan & Angelica Aviles-Rivero]

## [03463] Learning pair-wise homeomorphic image registration in a conformal-invariant hyperelastic setting

**Format** : Talk at Waseda University

**Author(s)** : Noémie DEBROUX (Université Clermont Auvergne)Jing Zou (The Hong Kong Polytechnic University)Lihao Liu (University of Cambridge)Angelica Aviles-Rivero (University of Cambridge)Jing Qin (The Hong Kong Polytechnic University)Carola-Bibiane Schönlieb (University of Cambridge)

**Abstract** : Deformable image registration is a fundamental task in medical image analysis and plays a crucial role in a wide range of clinical applications. Recently, deep learning-based approaches have been widely studied for deformable medical image registration and achieved promising results. However, existing deep learning image registration techniques

do not theoretically guarantee physically-meaningful transformations and usually require a lot of training data. In order to overcome these drawbacks, we propose a novel framework for pair-wise deformable image registration in a deep-learning framework. Firstly, we introduce a novel regulariser in the loss function based on conformal-invariant properties in a nonlinear elasticity setting. It theoretically guarantees that the obtained deformations are homeomorphisms and therefore preserve topology. Secondly, we boost the performance of our regulariser through coordinate MLPs, where one can view the to-be-registered images as continuously differentiable entities. We evaluate our model through extensive numerical experiments.

## [03252] Spherical Image Inpainting with Frame Transformation and Data-driven Prior Deep Networks

**Format** : Talk at Waseda University

**Author(s)** : Tieyong Zeng (The Chinese University of Hong Kong)

**Abstract** : Spherical image processing has been widely applied in many important fields. In this talk, we focus on the challenging task of spherical image inpainting with deep learning-based regularizer. We employ a fast directional spherical Haar framelet transform and develop a novel optimization framework based on a sparsity part\_2

assumption. Furthermore, by employing progressive encoder-decoder architecture, a new and better-performed deep CNN denoiser is carefully designed and works as an implicit regularizer. Finally, we use a plug-and-play method to handle the proposed optimization model, which can be implemented efficiently by training the CNN denoiser prior. Numerical experiments are conducted and show that the proposed algorithms can greatly recover damaged spherical images and achieve the best performance over purely using deep learning denoiser and plug-and-play model. This is a joint work with Jianfei Li, Chaoyan Huang, Raymond Chan, Han Feng, and Michael Ng.

## [05441] Learning to solve inverse problems with unsupervised nonlinear models

**Format :** Talk at Waseda University

**Author(s) :** Rihuan Ke (University of Bristol)Carola-Bibiane Schönlieb (University of Cambridge)

**Abstract :** Deep learning methods have recently demonstrated remarkable achievements in solving inverse problems. At the core of these methods lies the learning tasks of finding effective inverse problem solvers from a parameterised operator space, which is typically high dimensional. In the context of supervised learning, these learning tasks can be effectively tackled with sufficient supervised data, consisting of paired measurements and ground truth solutions. However, when the ground truth solutions are unknown, these learning tasks can be as challenging as solving the inverse problems themselves. In this talk, we present a hybrid method that addresses the learning tasks in an unsupervised learning setting for denoising and inverse problems more generally, where access to high-quality supervised data is restrictive or unavailable. We highlight a class of nonlinear operators that can be learned from noisy data and offer close approximations to the optimal solutions. Based on these nonlinear operators, we introduce a learning algorithm for solving inverse problems with limited knowledge of the underlying ground truth solutions and noise distributions.

## [04181] A learning framework for mapping problems via Quasiconformal geometry

**Author(s) :** Ronald Lok Ming LUI (The Chinese University of Hong Kong)Qiguang Chen (The Chinese University of Hong Kong)

**Abstract :** Many imaging problems can be formulated as a mapping problem. A general mapping problem aims to obtain an optimal mapping that minimizes an energy functional subject to the given constraints. Existing methods to solve the mapping problems are often inefficient and can sometimes get trapped in local minima. An extra challenge arises when the optimal mapping is required to be diffeomorphic. In this talk, we address the problem by proposing a deep-learning based framework based on the Quasiconformal (QC) Teichmüller theories. The main strategy is to learn the Beltrami coefficient (BC) that represents a mapping as the latent feature vector in the deep neural network. The BC measures the geometric distortions under the mapping. As such, the proposed network based on QC theories is explainable. Another crucial advantage of the proposed framework is that once the network is successfully trained, the optimized mapping corresponding to each input data information can be obtained in real time. In this talk, we will illustrate our framework by applying it to solve the diffeomorphic image registration problem. The developed network, called the quasiconformal registration network (QCRegNet), outperforms other state-of-the-art image registration models. This work is supported by HKRGC GRF (Project IDs: 14305919, 14306721, 14307622).

02349 (3/3) : 4D @E817 [Chair: Angelica Aviles Rivero & Raymond H Chan]

## [05328] Physics Informed Graph Transformer for PDEs

**Format :** Online Talk on Zoom

**Author(s) :** Andrey Bryutkin (University of Cambridge)Angelica Aviles-Rivero (University of Cambridge)Jiahao Huang (Imperial College London)

**Abstract :** In recent years, robust PDE solvers have become increasingly important, necessitating more input variety. The physics-informed graph transformer (PhysGPN) uses graphs to solve underlying problems described on an irregular grid and combines multiple parameter inputs of the PDE. It applies a transformer network to learn specific resemblances of data and additional inputs, which the PDE provides. The architecture is designed to be discretization invariant and flexible enough to handle irregular meshes. The PhysGPN offers several advantages over traditional numerical methods, including increased computational efficiency, reduced time needed for obtaining solutions, and increased robustness to additional noise. This can lead to various challenges and applications for the setup.

## [03627] Continuous U-Net: Faster, Greater and Noiseless

**Format :** Talk at Waseda University

**Author(s) :** Chun-Wun Cheng (City University of Hong Kong)Christina Runkel (University of Cambridge)Lihao Liu (University of Cambridge)Raymond Honfu Chan (City University of Hong Kong)Carola-Bibiane Schönlieb (University of Cambridge)Angelica Aviles-Rivero (University of Cambridge)

**Abstract :** Image segmentation is a fundamental task in image analysis and clinical practice. The current state-of-the-art techniques are based on U-shape type encoder-decoder networks with skip connections called U-Net. Despite the powerful performance reported by existing U-Net type networks, they suffer from several major limitations. These issues include the hard coding of the receptive field size, compromising the performance and computational cost, as well as the fact that they do not account for inherent noise in the data. They have problems associated with discrete layers, and do not offer any theoretical underpinning. In this work we introduce continuous U-Net, a novel family of networks for image segmentation. Firstly, continuous U-Net is a continuous deep neural network that introduces new dynamic blocks modelled by second order ordinary differential equations. Secondly, we provide theoretical guarantees for our network demonstrating faster convergence, higher robustness and less sensitivity to noise. Thirdly, we derive qualitative measures to tailor-made segmentation tasks. We demonstrate, through extensive numerical and visual results, that our model outperforms existing U-Net blocks for several medical image segmentation benchmarking datasets.

## [02370] Recent advances in Ultrasound Biomedical Imaging

**Session Time & Room :** 5B (Aug.25, 10:40-12:20) @D515

**Type :** Proposal of Minisymposium

**Abstract :** Medical Ultrasound Imaging is the most widespread real-time non-invasive imaging system, and it is based on the ability of human tissue to reflect the ultrasound signals sent by a probe. The fundamental challenges shared by Ultrasound Imaging applications are arguably to achieve higher image resolution and to get fast real-time acquisitions, in both 2D and 3D settings. Such issues must be addressed from both a theoretical viewpoint, by optimizing the modelling of the signal acquisition and formation process, and from a computational perspective. In this respect, recent advances in computing power and data storage have allowed the development of new algorithms and array designs for cutting-edge ultrasound machines.

This minisymposium aims to gather leading experts in Ultrasound Imaging along with young researchers to present their contributions on theoretical, computational, and industrial topics, with the leading idea of ultimately improving ultrasound signal analysis and image reconstruction beyond the state-of-the-art. The presented research topics range from spatial coherence and PSF approximation, to optimal 2D and 3D array design, and are relevant to a wide variety of mathematical, medical, and industrial applications.

**Organizer(s) :** Federico Benvenuto, Valentina Candiani

**Classification :** 92C55, 94A08, 68U10, 94A12, Biomedical Ultrasound Imaging

**Minisymposium Program :**

02370 (1/1) : 5B @D515 [Chair: Valentina Candiani]

## [05140] Applications of Spatial Coherence to Ultrasonic Imaging

**Format :** Talk at Waseda University

**Author(s) :** David Pierson Bradway (Duke University)Gregg Trahey (Duke University)Nick Bottenus (University of Colorado Boulder)Will Long (Duke University)James Long (Rice University)Katelyn Flint (Duke University)Matthew Huber (Duke University)

**Abstract :** Conventional pulse-echo ultrasound imaging relies primarily on signals' relative magnitudes and is limited in its ability to mitigate acoustic clutter and other types of image degradation. Advances in computing power have recently enabled an alternative data analysis method utilizing spatial coherence, a measure of the similarity of the signals received across an ultrasound array. The theory of spatial coherence and applications to diagnostic medical ultrasound imaging will be reviewed.

## [04772] A local space-invariant approximation for DAS Point Spread Function computation

**Format :** Talk at Waseda University

**Author(s) :** Chiara Razzetta (DIMA - Università di Genova)Valentina Candiani (University of Genoa)Federico Benvenuto ( DIMA - Università di Genova)Marco Crocco (Esaote S.p.A.)

**Abstract :** The Delay And Sum (DAS) algorithm is the standard technique for ultrasound image reconstruction, it is usually implemented on the hardware of the ultrasound device and it depends on several parameters set in the machine.

This makes it possible to produce real time images but at the same time it is a limitation in studying parameter optimization to obtain better reconstructions.

In this talk, we propose an approximation of the computation of the DAS algorithm by decomposing it into a sum of space-invariant operators by means of a partition of the unity.

This approximation allows parameter optimization algorithms to be applied to the DAS in order to increase the resolution of the reconstruction.

## [03464] Design and 3-D medical applications of 2-D ultrasound sparse arrays

**Format :** Talk at Waseda University

**Author(s) :** Alessandro Ramalli (University of Florence)

**Abstract :** The talk will report on the design methods that are currently used for the development of 2-D sparse arrays. Sample implementations of 2-D sparse arrays based on piezoelectric and capacitive micromachined ultrasonic transducer technologies will be presented. Finally, images and videos of (real-time) 2-D sparse array applications to 3-D flow imaging, super-resolution imaging, and high frame rate imaging will be shown.

## [04653] Recent advances in array and sequence design for 3D and high frame rate medical ultrasound imaging

**Format :** Online Talk on Zoom

**Author(s) :** Herve Liebgott (Université Lyon 1)

**Abstract :** Medical ultrasound imaging has been based for years on the transmission of short pulses inside a thin beam. While the beam sweeps over the whole medium, images are reconstructed by beamforming the raw radio-frequency signals. Following the emergence of compressed sensing, faster acquisition concepts based on coded excitations have been suggested. This talk will present some challenges raised by such approaches e.g. choice of the codes, the array, decoding, and image reconstruction algorithm, ...

# [02376] Recent Advances in Dynamic Games and Control Theory and Their Connection to Data Science

**Session Time & Room :**

02376 (1/2) : 5B (Aug.25, 10:40-12:20) @D502

02376 (2/2) : 5C (Aug.25, 13:20-15:00) @D502

**Type :** Proposal of Minisymposium

**Abstract :** Dynamic games and control theory involve the study of how multiple agents make decisions and interact strategically over time. These problems have traditionally been challenging to solve. This mini-symposium focuses on the latest developments in dynamic games and control theory enabled by data science. We will discuss how learning-based control theory has advanced the field, as well as the connection between reinforcement learning and dynamic games. Additionally, we will explore how these advances are enabling new applications in autonomous systems, networked systems, cyber-physical systems, and mathematical finance. This symposium will foster innovative interdisciplinary research that potentially can break new ground.

**Organizer(s) :** Quanyan Zhu, Maggie Cheng

**Classification :** 91Axx**Minisymposium Program :**

02376 (1/2) : 5B @D502 [Chair: Quanyan Zhu]

**[03672] The Role of Information Structure in Games and Learning****Format :** Talk at Waseda University**Author(s) :** Quanyan Zhu (New York University)

**Abstract :** The information structure of dynamic multi-agent systems plays a crucial role in determining the observation patterns of states, actions, and payoffs during interactions between agents. Differences in information structure can lead to surprising outcomes in a game. This talk aims to explore the role of information in dynamic games and learning. Specifically, we introduce the concept of the "price of information" and the "price of transparency" to quantify the gain or loss under different information patterns. We will discuss how information affects the strategic learning process, in which agents form beliefs based on their observations and generate policies based on those beliefs. Additionally, we will present how informational design can be used to incentivize agents and achieve the designer's goals at equilibrium in multi-agent systems.

**[02854] Optimal transaction mechanism for dynamic storage management game in smart grid****Format :** Talk at Waseda University**Author(s) :** Yasuaki Wasa (Waseda University)

**Abstract :** In this talk, we discuss an optimal transaction mechanism for a dynamic storage management game in smart grids in order to minimize the imbalance penalty charge of the grid in the wholesale electricity market. Our proposed mechanism is inspired by the primal-dual decomposition technique and the contract theory in economics. First, we present that the optimal power charge control profiles of the storage devices constitute a dynamic market equilibrium with a real-time pricing mechanism in a distributed fashion. Under the linear-quadratic dynamic grid model, the optimal design of the reference adjustment to modify the real-time pricing mechanism is analytically derived. The effectiveness of our proposed mechanism is also illustrated and discussed through simulation.

**[02858] Reinforcement Learning Algorithm for Mixed Mean Field Control Games****Format :** Online Talk on Zoom**Author(s) :** Jean-Pierre Fouque (University of California Santa Barbara)

**Abstract :** We present a new combined Mean Field Control Game (MFCG) problem which can be interpreted as a competitive game between collaborating groups and its solution as a Nash equilibrium between the groups. We propose a reinforcement learning algorithm to approximate the solution of such mixed Mean Field Control Game problems. We test the algorithm on benchmark linear-quadratic specifications for which we have analytic solutions.

Joint work with A. Angiuli, N. Detering, Mathieu Laurière, and J. Lin

**[02930] Recent Advances on Fractional Optimal Control Problems****Format :** Talk at Waseda University**Author(s) :** Jun Moon (Hanyang University)

**Abstract :** In this talk, we study recent results on fractional control problems. We first consider the fractional optimal control problem with terminal and running state constraints in finite dimensions. Then we study the fractional optimal control problem (without state constraints) in infinite dimensions described by fractional evolution equations. For both problems, we obtain the Pontryagin maximum principle, which constitutes the necessary condition for optimality.

02376 (2/2) : 5C @D502 [Chair: Maggie Cheng]

## [03245] Stabilizability of Nash equilibrium

**Format :** Talk at Waseda University

**Author(s) :** Renren Zhang (Shandong University)

**Abstract :** We investigate the stabilizability of Nash equilibrium of the game-based control system (GBCS), which was first introduced to model control systems whose structures involve rational agents. The stabilizability problem is whether the regulator can stabilize the system by regulating the Nash equilibrium formed by the agents. Some explicit conditions on the stabilizability of GBCS are given, by investigating the solvability relationship between the associated algebraic Riccati equations (AREs) and the algebraic Riccati inequalities (ARIs).

## [04475] Cooperation and Cost Sharing Problems in Supply Networks

**Format :** Talk at Waseda University

**Author(s) :** Sanjith Gopalakrishnan (McGill University) Sriram Sankaranarayanan (Indian Institute of Management, Ahmedabad)

**Abstract :** Across several contexts such as supply chain security or traceability, costly actions by firms can yield payoffs to other firms in the network. Such positive externalities imply network-wide cooperative strategies can yield improvements over firms independently choosing individually-rational actions. However, cooperation can be hindered by disagreements over cost-sharing arrangements. In this talk, we review two recent applications and develop a general framework to identify implementable cost sharing mechanisms that can sustain network-wide cooperative actions.

## [03268] Hodge allocation for cooperative rewards

**Format :** Online Talk on Zoom

**Author(s) :** Tongseok Lim (Purdue University)

**Abstract :** Lloyd Shapley's cooperative value allocation theory is a central concept in game theory that is widely used in various fields to allocate resources and assess individual contributions. The Shapley formula and axioms that characterize it form the foundation of the theory.

Shapley value can be assigned only when all players are assumed to eventually form the grand coalition. We discuss how to extend Shapley's theory to account for value allocation in every partial coalition state.

# [02386] Recent advances on theory and algorithms in deep learning applications

**Session Time & Room :**

02386 (1/2) : 4E (Aug.24, 17:40-19:20) @E817

02386 (2/2) : 5B (Aug.25, 10:40-12:20) @E817

**Type :** Proposal of Minisymposium

**Abstract :** In recent years, supervised and unsupervised learning models based on deep neural networks play an increasingly important role in many directions, such as approximating continuous functions, constructing image models, and solving inverse problems. Meanwhile, many theoretical results are carried out to study the approximation and training properties of these approaches. This mini-symposium will bring together researchers in different areas to discuss recent advances in training algorithms and model applications, as well as relevant theoretical analysis. The aim is to assemble new understandings of the efficiency and limitation of deep learning models through the intersection discussion.

**Organizer(s) :** Yongqiang Cai, Qiaoqiao Ding

**Classification :** 68T07

**Minisymposium Program :**

02386 (1/2) : 4E @E817 [Chair: Yongqiang Cai]

## [03440] Vanilla Feedforward Neural Networks as a Discretization of Dynamical Systems

**Format :** Talk at Waseda University

**Author(s) :** Yongqiang Cai (Beijing Normal University)

**Abstract :** Deep learning has made significant progress in the fields of data science and natural science. Some studies have linked deep neural networks to dynamical systems, but the network structure is restricted to a residual network. It is known that residual networks can be regarded as a numerical discretization of dynamical systems. In this talk, we consider the traditional network structure and prove that vanilla feedforward networks can also be used for the numerical discretization of dynamical systems, where the width of the network is equal to the dimensions of the input and output. Our proof is based on the properties of the leaky-ReLU function and the numerical technique of the splitting method for solving differential equations. Our results could provide a new perspective for understanding the approximation properties of feedforward neural networks.

## [03441] Phase Diagram of Initial Condensation for Two-layer Neural Networks

**Format :** Talk at Waseda University

**Author(s) :** Zhengan Chen (Shanghai Jiao Tong University)Yuqing Li (Shanghai Jiao Tong University)Tao Luo (Shanghai Jiao Tong University)Zhangchen Zhou (Shanghai Jiao Tong University)Zhiqin Xu (Shanghai Jiao Tong University)

**Abstract :** The phenomenon of distinct behaviors exhibited by neural networks under varying scales of initialization remains an enigma in deep learning research. In this paper, based on the earlier work by Luo et al.~\cite{luo2021phase}, we present a phase diagram of initial condensation for two-layer neural networks. Condensation is a phenomenon wherein the weight vectors of neural networks concentrate on isolated orientations during the training process, and it is a feature in non-linear learning process that enables neural networks to possess better generalization abilities. Our phase diagram serves to provide a comprehensive understanding of the dynamical regimes of neural networks and their dependence on the choice of hyperparameters related to initialization. Furthermore, we demonstrate in detail the underlying mechanisms by which small initialization leads to condensation at the initial training stage.

## [03386] Robust Full Waveform Inversion: A Source Wavelet Manipulation Perspective

**Format :** Talk at Waseda University

**Author(s) :** Chenglong Bao (Tsinghua University)Lingyun Qiu (Tsinghua University)Rongqian Wang (Tsinghua University)

**Abstract :** Full-waveform inversion (FWI) is a powerful tool for high-resolution subsurface parameter reconstruction. Due to the existence of local minimum traps, the success of the inversion process usually requires a good initial model. Our study primarily focuses on understanding the impact of source wavelets on the landscape of the corresponding optimization problem. We thus introduce a decomposition scheme that divides the inverse problem into two parts. The first step transforms the measured data into data associated with the desired source wavelet. Here, we consider inversions with known and unknown sources to mimic real scenarios. The second subproblem is the conventional full waveform inversion, which is much less dependent on an accurate initial model since the previous step improves the misfit landscape. A regularized deconvolution method and a convolutional neural network are employed to solve the source transformation problem. Numerical experiments on the benchmark models demonstrate that our approach improves the gradient's quality in the subsequent FWI and provides a better inversion performance.

## [02945] Learning robust imaging model with unpaired data

**Format :** Talk at Waseda University

**Author(s) :** Chenglong Bao (Tsinghua University)

**Abstract :** In this talk, in the unpaired data regime, we discuss our recent progress in building AI-aided robust models and their applications in image processing. Leveraging the Bayesian inference framework, our model combines classical mathematical modeling and deep neural networks to improve interpretability. Experimental results on various real datasets validate the advantages of the proposed methods.

## [03329] Generative Models Based Statistical Priors for Compressive Sensing and Medical Imaging

**Format :** Talk at Waseda University

**Author(s) :** Jiulong Liu (Academy of Mathematics and Systems Science, Chinese Academy of Sciences)

**Abstract :** Sparsity is a mathematically elegant tool for reducing the sampling rate for compressive sensing reconstruction and thereby its applications are also extended to many underdetermined imaging systems, such as MRI and CT. However, with the development of deep learning, there are many methods proposed to learn data representation and they are shown to be more efficient in signal and image processing. In order to efficiently and stably solve the under-determined and ill-conditioned inverse problems with fewer measurements, we established compressive sensing reconstruction methods using generative priors which are shown much more efficient than the traditional priors or some other data-driven priors. In this talk, I will introduce some of these methods and present our recent results for MRI reconstruction, phase retrieval, and some other nonlinear inverse problems.

## [03483] Normalizing-flows based design of experiments for failure probability estimation

**Format :** Talk at Waseda University

**Author(s) :** Hongqiao Wang (Central South University)

**Abstract :** Failure probability estimation problem is an crucial task in engineering. In this work we consider this problem in the situation that the underlying computer models are extremely expensive, which often arises in the practice, and in this setting, reducing the calls of computer model is of essential importance. We formulate the problem of estimating the failure probability with expensive computer models as an sequential experimental design for the limit state (i.e., the failure boundary) and propose a series of efficient adaptive design criteria to solve the design of experiment (DOE). In particular, the proposed method employs the deep neural network (DNN) as the surrogate of limit state function for efficiently reducing the calls of expensive computer experiment. A map from the Gaussian distribution to the posterior approximation of the limit state is learned by the normalizing flows for the ease of experimental design. Three normalizing-flows-based design criteria are proposed in this work for deciding the design locations based on different assumption of generalization error. The accuracy and performance of the proposed method is demonstrated by both theory and practical examples.

## [03477] Unsupervised learning driven by Langevin dynamics and its applications to inverse problems

**Format :** Talk at Waseda University

**Author(s) :** Ji Li (Capital Normal University)

**Abstract :** From the Bayesian view, the key component of image restoration is to estimate the posterior distribution. Generally, the sampling from posterior distribution is intractable. To this end, there have been some variational approaches to approximate the posterior distribution using a proxy distribution. In this talk, we first review the Langevin dynamics as an effective sampler for a given distribution. Then we apply it or embed it to the unsupervised learning solution to two image restoration problems with slight modifications.

## [03450] Self-supervised Deep learning Methods in Imaging

**Format :** Online Talk on Zoom

**Author(s) :** Tongyao Pang (National University of Singapore)

**Abstract :** In this talk, I will share our recent research on using self-supervised deep learning techniques for image reconstruction. Deep learning has recently become a powerful tool in image restoration but it requires a large amount of paired training data. Our proposed self-supervised methods alleviate this requirement while still achieving comparable performance to supervised learning. Our methods are designed to find the minimum mean-squared error (MMSE) solution from a Bayesian inference perspective.

# [02387] Recent Advances on Distributed Optimization

**Session Time & Room :** 2E (Aug.22, 17:40-19:20) @E804

**Type :** Proposal of Minisymposium

**Abstract :** Distributed algorithms have emerged as a key driving force in solving large-scale optimization and machine learning problems, with a wide range of applications spanning from training deep neural network models over GPU clusters to boosting edge intelligence over networks consisting of cellphones, tablets, and wearables. In this minisymposium, we will review recent advances in distributed optimization, with a focus on state-of-the-art sample and communication complexities, novel communication compression techniques, and new decentralized or federated algorithms. By bringing together leading researchers and practitioners in this field, we hope to identify key challenges and opportunities for advancing distributed optimization.

**Organizer(s) :** Kun Yuan, Shi Pu

**Classification :** 68W15, 90C06, 90C30

**Minisymposium Program :**

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02387 (1/1) : 2E @E804

## [03522] Optimal Gradient Tracking for Decentralized Optimization

**Format :** Talk at Waseda University

**Author(s) :** Ming Yan (The Chinese University of Hong Kong, Shenzhen)

**Abstract :** We focus on solving the decentralized problem over a network. Assuming smoothness and strong convexity, we propose Optimal Gradient Tracking (OGT), which simultaneously achieves the optimal gradient computation complexity and communication complexity. Its development involves two building blocks that are of independent interest. The first is the decentralized gradient tracking method, SSGT, which achieves optimal gradient computation. The second is a loopless method that achieves similar performance as Chebyshev acceleration.

## [03541] Optimal Complexity in Distributed Learning with Communication Compression

**Format :** Talk at Waseda University

**Author(s) :** Yutong He (Peking University)Xinmeng Huang (University of Pennsylvania)Wotao Yin (Alibaba (US) Group)Kun Yuan (Peking University)

**Abstract :** Recent advances in distributed optimization and learning have shown that communication compression is one of the most effective means of reducing communication. While there have been many results on convergence rates under communication compression, a theoretical lower bound is still missing.

Analyses of algorithms with communication compression have attributed convergence to two abstract properties: the unbiased property or the contractive property. In this talk, we consider distributed stochastic algorithms for minimizing smooth convex and non-convex objective functions under communication compression. We establish convergence lower bounds for algorithms whether using unbiased or contractive compressors. To close the gap between the lower bound and the existing upper bounds, we further propose an algorithm, NEOLITHIC, which almost reaches our lower bound (up to logarithm factors) under mild conditions. The experimental results validate our findings.

## [03556] Asymptotic Network Independence in Distributed Stochastic Gradient Methods

**Format :** Talk at Waseda University

**Author(s) :** Shi Pu (The Chinese University of Hong Kong, Shenzhen)

**Abstract :** We discuss the so-called asymptotic network independence property in distributed stochastic optimization, which is achieved whenever a distributed method executed over a network of  $n$  nodes asymptotically converges to the optimal solution at a comparable rate to a centralized method with the same computational power as the entire network; it is as if the network is not even there! We explain this property through examples involving the training of ML models and present a short mathematical analysis. We also discuss the transient times for

distributed stochastic gradient methods to achieve network independent convergence rates. Finally, we introduce some recent works on distributed random reshuffling (RR) methods.

## [03570] Unified and Refined Analysis of Decentralized Optimization and Learning Algorithms

**Format :** Talk at Waseda University

**Author(s) :** Sulaiman A Alghunaim (Kuwait University)

**Abstract :** Decentralized multi-agent optimization is a powerful paradigm with numerous applications in learning and engineering design. In these setups, a network of agents is linked by a graph, and agents are only allowed to share information locally. Through localized interactions, they seek the minimizer of a global optimization problem. In decentralized consensus problems, the agents are linked by a common consensus variable on which they must agree.

This talk will present a unified and improved analysis for decentralized consensus optimization methods. We demonstrate how the analysis of several state-of-the-art bias-correction decentralized methods, such as EXTRA, Exact-Diffusion, NIDS, and Gradient-Tracking methods, can be unified by a decentralized algorithmic framework that encompasses these methods. We develop a novel analysis technique that establishes the framework's convergence under nonconvex, convex, and strongly convex objectives. We provide refined and improved convergence rate bounds. The analysis reveals important characteristics for these methods, such as how their performances are influenced by network graph.

## [02392] Low-Rank Models in Data Science

**Session Time & Room :**

02392 (1/3) : 2C (Aug.22, 13:20-15:00) @G306

02392 (2/3) : 2D (Aug.22, 15:30-17:10) @G306

02392 (3/3) : 2E (Aug.22, 17:40-19:20) @G306

**Type :** Proposal of Minisymposium

**Abstract :** Due to their simplicity and versality that ranges from genomics data to computational physics, recommender systems and unsupervised learning, low-rank matrix models have emerged as a powerful tool in data science. However, only few related computational problems admit closed-form solutions. Convex or non-convex potentially non-smooth optimization problems with different statistical properties can be used to overcome involving computational challenges.

This minisymposium intends to shed light on recent advances in structured numerical optimization for low-rank models and their statistical and information theoretical properties by bringing together experts from applied mathematics and engineering working these topics, providing a forum for future collaborations.

**Organizer(s) :** Christian Kümmerle, Johannes Maly, Dominik Stöger

**Classification :** 15A83, 65F55, 65K10, 90C26

**Minisymposium Program :**

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02392 (1/3) : 2C @G306 [Chair: Christian Kümmerle]

## [02769] Low-rank models in data science: Applications and optimization challenges

**Format :** Online Talk on Zoom

**Author(s) :** Dominik Stöger (KU Eichstätt-Ingolstadt)

**Abstract :** Low-rank matrix models have emerged as a powerful tool in data science with applications ranging from recommender systems to computational physics. In this overview talk, we first highlight some applications where low-rank models arise. Next, we discuss which statistical and optimization challenges arise. Moreover, we highlight several advances which have been made in recent years to circumvent these issues.

## [05455] Low Rank Matrix Recovery from Column-wise Projections: Fast and Communication-Efficient Solutions

**Format :** Online Talk on Zoom

**Author(s) :** Namrata Vaswani (Iowa State University)

**Abstract :** We study the following lesser-known low rank (LR) recovery problem: recover an  $n \times q$  rank- $r$  matrix,  $X^* = [x_1^*, x_2^*, \dots, x_q^*]$ , with  $r \ll \min(n, q)$ , from  $m$  independent linear projections of each of its  $q$  columns, i.e., from  $y_k := A_k x_k^*$ ,  $k \in [q]$ , when  $y_k$  is an  $m$ -length vector with  $m < n$ . The matrices  $A_k$  are known and mutually independent for different  $k$ . We introduce a novel gradient descent (GD) based solution called AltGD-Min. We show that, if the  $A_k$ 's are i.i.d. with i.i.d. Gaussian entries, and if the right singular vectors of  $X^*$  satisfy the incoherence assumption, then  $\epsilon$ -accurate recovery of  $X^*$  is possible with order  $(n + q)r^2\log(1/\epsilon)$  total samples and order  $mqr\log(1/\epsilon)$  time. Compared with existing work, this is the fastest solution, and in most practical settings, it also has the best sample complexity. For a federated implementation, it is also communication-efficient with a cost of only order  $nr$  per node per iteration.

A simple extension of AltGD-Min also provably solves the LR Phase Retrieval problem, which is a magnitude-only measurements' extension of the above problem.

## [04491] Tensor-Norm Approaches to Low-Rank Matrix Recovery by Convex Program

**Format :** Online Talk on Zoom

**Author(s) :** Kiryung Lee (Ohio State University)

**Abstract :** Low-rank models have been shown effective for solving various inverse problems from classical system identification to modern matrix completion and sketching in signal processing and statistics. If each observation is a linear combination of a subset of matrix entries, the reconstruction is feasible only for a class of matrices incoherent to the measurement process. We propose an estimator that prefers a solution with low rankness and incoherence by a regularizer given by a pair of norms on the tensor product of two Banach spaces. The resulting optimization is cast as a convex semidefinite program and provides a near-optimal error matching the corresponding minimax bound in a low signal-to-noise ratio regime. We illustrate the efficacy of the estimator over selected applications in signal processing. We also present a scalable numerical optimization algorithm and study its empirical performance over large-scale synthesized data.

## [04277] Algorithmic approaches to recovering sparse and low-rank matrices

**Format :** Talk at Waseda University

**Author(s) :** Johannes Maly (Ludwig-Maximilians-Universität München)

**Abstract :** In this talk, I consider the problem of recovering an unknown sparse and low-rank matrix  $X$  from measurements gathered in a linear measurement process. I discuss the challenges that come with leveraging several structures simultaneously and present two new algorithmic strategies to efficiently approach the problem. Both strategies come with local convergence guarantees.

02392 (2/3) : 2D @G306 [Chair: Johannes Maly]

## [03939] Bures-Wasserstein Methods in Matrix Recovery

**Format :** Talk at Waseda University

**Author(s) :** Tyler Maunu (Brandeis University)

**Abstract :** We revisit the problem of recovering a positive semidefinite matrix from a linear map using tools from optimal transport. More specifically, we connect a variational formulation of this problem to the computation of Wasserstein barycenters. This new perspective enables the development of efficient first-order geometric methods. Experiments demonstrate the advantages of our new methodology over existing methods. We also discuss extensions to recovery in other settings of restricted positive semidefinite matrices.

## [05442] Improved Global Guarantees for Low-Rank Models via Rank Overparameterization

**Format :** Talk at Waseda University

**Author(s) :** Richard Y Zhang (University of Illinois at Urbana-Champaign)

**Abstract :** We consider minimizing a twice-differentiable,  $L$ -smooth, and  $\mu$ -strongly convex objective  $\phi$  over an  $n \times n$  positive semidefinite matrix  $M \succeq 0$ , under the assumption that the minimizer  $M^*$  has low rank  $r^* \ll n$ . Following the Burer-Monteiro approach, we instead minimize the nonconvex objective  $f(X) = \phi(XX^T)$  over a factor matrix  $X$  of size  $n \times r$ . This substantially reduces the number of variables from  $O(n^2)$  to as few as  $O(n)$  and also enforces positive semidefiniteness for free, but at the cost of giving up the convexity of the original problem. In this talk, we prove that if the search rank  $r \geq r^*$  is overparameterized by a constant factor with respect to the true rank  $r^*$ , namely as in  $r > \frac{1}{4}(L/\mu - 1)^2 r^*$ , then despite nonconvexity, local optimization is guaranteed to globally converge from any initial point to the global optimum. This significantly improves upon a previous rank overparameterization threshold of  $r \geq n$ , which is known to be sharp if  $\phi$  is allowed to be nonsmooth and/or non-strongly convex, but would increase the number of variables back up to  $O(n^2)$ . Conversely, without rank overparameterization, we prove that such a global guarantee is possible if and only if  $\phi$  is almost perfectly conditioned, with a condition number of  $L/\mu < 3$ . Therefore, we conclude that a small amount of overparameterization can lead to large improvements in theoretical guarantees for the nonconvex Burer-Monteiro factorization.

## [04377] Tensor Completion via Tensor Train Based Low-Rank Quotient Geometry under a Preconditioned Metric

**Format :** Talk at Waseda University

**Author(s) :** Ke Wei (Fudan University)

**Abstract :** Low-rank tensor completion problem is about recovering a tensor from partially observed entries. We consider this problem in the tensor train format and extend the preconditioned metric from the matrix case to the tensor case. The first-order and second-order quotient geometry of the manifold of fixed tensor train rank tensors under this metric is studied in detail. Algorithms, including Riemannian gradient descent, Riemannian conjugate gradient, and Riemannian Gauss-Newton, have been proposed for the tensor completion problem based on the quotient geometry. It has also been shown that the Riemannian Gauss-Newton method on the quotient geometry is equivalent to the Riemannian Gauss-Newton method on the embedded geometry with a specific retraction. Empirical evaluations on random instances as well as on function-related tensors show that the proposed algorithms are competitive with other existing algorithms in terms of completion ability, convergence performance, and completion quality.

## [04975] Iteratively Reweighted Least Squares for Low-Rank Optimization: Optimality & Convergence Rates

**Format :** Talk at Waseda University

**Author(s) :** Christian Kümmerle (University of North Carolina at Charlotte)

**Abstract :** Convex or non-convex matrix functions such as Schatten- $p$  (quasi-)norms have been successfully used as surrogates of the rank objective. Iteratively Reweighted Least Squares (IRLS) has emerged as a suitable algorithmic framework to scalably optimize such rank surrogates. We review the formulation, optimality and empirical data-efficiency of MatrixIRLS. We show that the algorithm, which optimizes Schatten-type objectives, exhibits a local superlinear convergence rate with a large basin of attraction, and linear convergence rates in the convex case.

## [04701] Multi-window Gabor phase retrieval

**Format :** Online Talk on Zoom

**Author(s) :** Palina Salanevich (Utrecht University)

**Abstract :** Phase retrieval is the non-convex inverse problem of signal reconstruction from its intensity measurements that is motivated by practical applications. In the talk, we are going to focus on phase retrieval with multi-window Gabor frames, where the measurement vectors follow time-frequency structure natural for imaging and acoustics. We will propose an explicit construction of such frames and show that for them phase retrievability can be achieved with a close to optimal number of phaseless measurements.

## [02396] Recent Advances on Polynomial System Solving

**Session Time & Room :**

02396 (1/3) : 1C (Aug.21, 13:20-15:00) @G305

02396 (2/3) : 1D (Aug.21, 15:30-17:10) @G305

02396 (3/3) : 1E (Aug.21, 17:40-19:20) @G305

**Type :** Proposal of Minisymposium

**Abstract :** Polynomial systems are fundamental mathematical objects in algebraic geometry, automated geometric reasoning, cryptography, coding theory, biology, and many other areas of science and engineering, and thus finding the solutions of polynomial systems algorithmically is also of both theoretical and practical importance. This minisymposium aims at bringing together interested researchers to present and to discuss recent work and progress on the theories, algorithms, software, and applications of solving polynomial systems.

**Organizer(s) :** Deepak Kapur, Chenqi Mou

**Classification :** 13P15, 68W30, 13P10, 14Q30

**Minisymposium Program :**

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02396 (1/3) : 1C @G305 [Chair: Changbo Chen]

## [03796] Polynomial System Solving in a Nutshell

**Format :** Talk at Waseda University

**Author(s) :** Chenqi Mou (Beihang University)

**Abstract :** In this introductory talk of the minisymposium “Recent Advances on Polynomial System Solving”, I will give a brief overview of the problem of solving polynomial systems, including its theories, methods, softwares, and applications. In particular, basic concepts of three typical methods of Gröbner bases, triangular decomposition, and homotopy continuation for solving polynomial systems will be presented, serving as an introduction of other talks in this minisymposium to a wider audience of different backgrounds.

## [04394] Signature-based algorithm and change of ordering for Groebner basis

**Format :** Talk at Waseda University

**Author(s) :** Masayuki Noro (Rikkyo University)

**Abstract :** Although the termination is not guaranteed, signature-based algorithm under non-compatible term orderings may give good performance for computing Groebner bases. In such cases, we can apply the notion of Hilbert function for guaranteeing the termination. The Hilbert function is given by a Groebner basis with respect to another term ordering and thus this algorithm is a kind of change of ordering. We compare its performance with the usual Hilbert driven algorithm.

## [03913] Dimension results for polynomial systems over complete toric varieties

**Format :** Talk at Waseda University

**Author(s) :** Matías Bender (INRIA - CMAP, École polytechnique, IPP)Pierre-Jean Spaenlehauer (INRIA Nancy)

**Abstract :** A common computational approach to study affine varieties is to first homogenize the input defining equations. Among other reasons, we do so because the new equations have an associated grading that allows us to reduce our computations to a linear algebra problem. However, the homogenization process might introduce higher components at infinity, changing drastically the geometry of the affine object that we want to study. This is what happens when we homogenize, in the classical sense, sparse polynomials. To overcome this issue, a possible approach is to homogenize the input equations, using their Newton polytopes, over a Cox ring or a polytopal graded subring of it. However, other simpler homogenizations might be possible. In this work, we prove a combinatorial criterion to decide when a candidate homogenization is good, in the sense that it does not introduce higher components at infinity. Additionally, we use our criterion to decide which families of degrees on polytopal algebras lead to regular sequences.

## [03633] On the computation of staggered linear bases

**Format :** Talk at Waseda University

**Author(s) :** Amir Hashemi (Isfahan University of Technology)Hans Michael Moller (Technical University Dortmund)

**Abstract :** Grobner bases are a powerful tool in polynomial ideal theory with many applications in various areas of science and engineering. Considering an ideal as a vector space, we investigate for such an ideal a particular linear basis, so-called staggered linear basis, which contains a Grobner basis as well. This notion was first introduced by Gebauer and Moller in 1988, however the algorithm that they described for computing these bases was not complete. In this talk, we present a simple and efficient algorithm to compute an staggered linear basis. The new framework is equipped with some novel criteria (including both Buchberger's criteria) to detect superfluous reductions. Finally, we discuss the efficiency of this algorithm compared to the existing methods using a set of benchmark polynomials.

02396 (2/3) : 1D @G305 [Chair: Chenqi Mou]

## [03688] Square-Free Pure Triangular Decomposition of Zero-Dimensional Polynomial Systems

**Format :** Talk at Waseda University

**Author(s) :** Haokun Li (Peking University)Bican Xia (Peking University)Tianqi Zhao (Peking University)

**Abstract :** The concepts of pure chains and square-free pure triangular decomposition (SFPTD) of zero-dimensional polynomial systems are defined. We propose an algorithm for computing SFPTD and prove its arithmetic complexity can be single exponential in the square of the number of variables. We show experimentally that, on most examples in the literature, the algorithm is more efficient than a triangular-decomposition method in Maple, and the real solution isolation method based on SFPTD is very efficient.

## [05286] On the bit complexity of roadmap algorithms

**Format :** Talk at Waseda University

**Author(s) :** Eric Schost (University of Waterloo)

**Abstract :** Roadmaps were introduced by Canny in order to reduce connectivity queries on semi-algebraic sets to similar questions on curves. In the last ten years, with Mohab Safey El Din, we proposed randomized algorithms with an improved complexity - in an algebraic cost model; the bit-complexity analysis remained to be done. I will report on recent work done in this direction with Jesse Elliott.

## [03750] Solving semi-algebraic systems arising in applications

**Format :** Talk at Waseda University

**Author(s) :** Changbo Chen (Chongqing Institute of Green and Intelligent Technology, Chinese Academy of Sciences)

**Abstract :** Semi-algebraic systems, which are systems consisting of polynomial equations and inequalities, naturally appear in many applications. To solve them efficiently, it is important to exploit their particular structures. In this talk, I will present specialized algorithms designed for solving semi-algebraic systems arising in

several applications, namely computing the steady states of parametric biological systems, automatic parallelization of loops, and detecting quantum correlations.

### [04993] Root Separation Bounds

**Format :** Talk at Waseda University

**Author(s) :** Vikram Sharma (The Institute of Mathematical Sciences Chennai)

**Abstract :** Root separation bounds are a classical topic in algebraic number theory. They also play an important role in the analysis of algorithms for finding the roots of polynomials. In this talk, we will start with some classical results of Mignotte and Davenport and trace the recent development that has occurred in this area.

02396 (3/3) : 1E @G305

## [02402] Numerical methods for a class of time-dependent PDEs

**Session Time & Room :**

02402 (1/2) : 1C (Aug.21, 13:20-15:00) @E704

02402 (2/2) : 1D (Aug.21, 15:30-17:10) @E704

**Type :** Proposal of Minisymposium

**Abstract :** Many phenomena and problems in modern science, technology and engineering can be described by partial differential equations. For example, the Gross-Pitaevskii equation under a rotational frame, the nonlinear Klein-Gordon-Schr{<sup>o</sup>}dinger equations in the nonrelativistic limit regime, Poisson-Nernst-Planck systems, etc. It is significant to design efficient numerical methods to solve the above PDEs with numerical analysis and provide an intuitive view for physical phenomena. The main purpose of this mini-symposium is to discuss recent developments of the numerical methods for solving time-dependent PDEs.

**Organizer(s) :** Fenghua Tong, Yong Wu, Zhongyang Liu, Xuanxuan Zhou

**Classification :** 65M70, 65M12, 65N22

**Minisymposium Program :**

02402 (1/2) : 1C @E704

## [02681] Unconditionally MBP-preserving linear schemes for conservative Allen-Cahn equations

**Format :** Talk at Waseda University

**Author(s) :** Jingwei Li (Lanzhou University)

**Abstract :** The maximum bound principle MBP, is an important property for semilinear parabolic equations, in the sense that the time-dependent solution of the equation with appropriate initial and boundary conditions and nonlinear operator preserves for all time a uniform pointwise bound in absolute value. It has been a challenging problem to design unconditionally MBP-preserving high-order accurate time-stepping schemes for these equations. Du Qiang et al have established a unified analytical framework on the MBP preserving scheme for the semilinear parabolic equations which in this talk will be extended to conservative Allen-Cahn equation with the introduced Lagrange multiplier enforcing the mass conservation. Some sufficient conditions on the nonlinear potentials will be given under which the MBP holds and then the stabilized exponential time differencing scheme is proposed for time integration, which are linear schemes and unconditionally preserve the MBP in the time discrete level. Convergence of these schemes is analyzed as well as their energy stability. Various two and three dimensional numerical experiments are also carried out to validate the theoretical results and demonstrate the performance of the proposed schemes. These work are joint with Cai Yongyong, Feng Xinlong, Huang Qiumei, Jiang Kun, Ju Lili, Li Xiao, Lan Rihui et al.

## [02717] Uniformly accurate nested Picard iterative integrators for the Klein-Gordon-Schr"oedinger equation in the nonrelativistic regime

**Format :** Online Talk on Zoom

**Author(s) :** xuanxuan zhou (beijing normal university)

**Abstract :** We establish a class of uniformly accurate nested Picard iterative integrator (NPI) Fourier pseudospectral methods for the nonlinear Klein-Gordon-Schr"oedinger equation (KGS) in the nonrelativistic regime, involving a dimensionless parameter  $\epsilon \ll 1$  inversely proportional to the speed of light. Actually, the solution propagates waves in time with  $O(\epsilon^2)$  wavelength when  $0 < \epsilon \ll 1$ , which brings significant difficulty in designing accurate and efficient numerical schemes. The NPI method is designed by separating the oscillatory part from the non-oscillatory part, and integrating the former exactly. Based on the Picard iteration, the NPI method can be applied to derive arbitrary higher-order methods in time with optimal and uniform accuracy (w.r.t.  $\epsilon \in (0, 1]$ ), and the corresponding error estimates are rigorously established. In addition, the practical implementation of the second-order NPI method via Fourier pseudospectral discretization is clearly demonstrated, with extensions to the third order NPI. Some numerical examples are provided to support our theoretical results and show the accuracy and efficiency of the proposed schemes.

## [02550] Structure-preserving scheme for the PNP equations

**Format :** Talk at Waseda University

**Author(s) :** Fenghua Tong (Beijing Normal University)

**Abstract :** Poisson-Nernst-Planck system is a macroscopic model to describe the ion transport process. We propose a novel method to construct the positivity preserving and mass conservation scheme for the Poisson-Nernst-Planck equations. The method is based on the discrete  $L_h^2$  or  $H_h^1$  projection strategy in which the solution projected from the intermediate solution computed by semi-implicit scheme inherits the positivity preservation and mass conservation with negligible additional computational cost resulting from the nonlinear algebraic equation.

## [02553] Numerical simulation of rotational nonlinear Schrodinger equations with attractive interactions

**Format :** Talk at Waseda University

**Author(s) :** Yong Wu (Beijing Normal University)

**Abstract :** We consider the focusing Schr"oedinger equation with rotation and numerically simulate the ground state and dynamic properties. We take the gradient flow with Lagrange multiplier (GFLM) method to compute the ground state and time splitting pseudospectral method to simulate dynamics. We numerically verify the nonexistence of vortices in harmonic symmetry potential and analytically derive that the symmetric state energy ( $m=0$ ) is always lower than the central vortex state energy ( $m=1$ ) when the attractive interaction is sufficiently small. For dynamics properties, we mainly simulated the condensate widths, a stationary state with a shifted center and stability of central vortex states and found that the conclusion is completely consistent with the repulsive interaction. Finally, we numerically simulate the global existence and finite time blow-up of solution in mass-supercritical case.

02402 (2/2) : 1D @E704

## [02622] IMPROVED UNIFORM ERROR BOUNDS OF THE TIME-SPLITTING HERMITE SPECTRAL METHODS FOR THE LONG-TIME GROSS PITAEVSKII EQUATION WITH WEAK NONLINEARITY

**Format :** Online Talk on Zoom

**Author(s) :** Zhongyang Liu (Beijing Normal University)

**Abstract :** The aim of this research is to carry out a improved uniform error bounds for the Strang splitting Hermite pseudospectral methods for the long-time dynamics of the time-dependent Gross-Pitaevskii equation (GPE) with weak nonlinearity, while the nonlinearity strength is characterized by  $\epsilon^2$  with a dimensionless parameter  $\epsilon \in (0, 1]$ , for the long time dynamics up to the time at  $O(\epsilon^{-2})$ . We derive a improved uniform  $H_A^1$  error bounds for full discretizations of the one-dimensional GPE by the Strang splitting Hermite pseudospectral method as  $O(N^{2/3 - \frac{m}{2}} + \epsilon^2 \tau^2)$  up to the time at  $O(1/\epsilon^2)$ . The error bounds are uniformly accurate up to the time at  $O(\epsilon^{-2})$  and uniformly valid for  $\epsilon$ .

# [02404] New Trends in Hierarchical Variational Inequalities and Optimization Problems

## Session Time & Room :

02404 (1/4) : 1C (Aug.21, 13:20-15:00) @E606  
 02404 (2/4) : 1D (Aug.21, 15:30-17:10) @E606  
 02404 (3/4) : 1E (Aug.21, 17:40-19:20) @E606  
 02404 (4/4) : 2C (Aug.22, 13:20-15:00) @E606

## Type : Proposal of Minisymposium

**Abstract :** It is well known that the bilevel programming problem has been widely investigated in the literature due to its applications in mechanics, network designs and so on. In particular, if the upper-level problem is a variational inequality problem and the lower-level is a fixed-point set of an operator, then such a bilevel problem is known as a hierarchical variational inequality problem. The signal recovery, beamforming and power control problems can be modelled as hierarchical variational inequality problems. This minisymposium will promote a few scholars to look into new trends in hierarchical variational inequalities and optimization problems together, and provide an opportunity to explore the latest developments.

## Organizer(s) : Lu-Chuan Ceng

**Classification :** 65K15, 47H05, 47H10, 65Y05, 68W25

## Minisymposium Program :

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02404 (1/4) : 1C @E606

## [03031] Self-adaptive subgradient extragradient method with extrapolation procedure for MSVIs

### Author(s) : Lu-Chuan Ceng (Shanghai Normal University)

**Abstract :** This article introduces a self-adaptive subgradient extragradient process with extrapolation to solve a bilevel split pseudomonotone variational inequality with common fixed points constraint of finite nonexpansive mappings. The proposed rule exploits the strong monotonicity of one operator at the upper level and the pseudomonotonicity of another mapping at the lower level. The strong convergence result for the proposed algorithm is established. A numerical example is used to demonstrate the viability of the proposed rule.

## [03050] Subgradient-extragradient method for SEP, VIP and FPP of multi-valued mapping

### Author(s) : Yun-shui Liang (Yichun Vocational Technique College)

**Abstract :** In this paper, via a subgradient extragradient implicit rule, we introduce a new iterative algroithm for solving split equilibrium problems, variational inequality problem and fixed point problem of nonspreadng multi-valued mapping in Hilbert space. We show that the iteration converges strongly to a common solution of the considered problems. Our results extend and improve some well-known results in the literature. Finally, a numerical example is provided to verify the validity of the proposed algorithm.

## [03061] Modified subgradient-extragradient method for monotone-bilevel-equilibria with VIP and CFPP constraints

### Author(s) : Hui-ying Hu (shanghai normal university)

**Abstract :** In a real Hilbert space, let GSVI and CFPP represent a general system of variational inequalities and a common fixed point problem of a countable family of nonexpansive mappings and an asymptotically nonexpansive mapping, respectively. In this paper, we introduce and analyze two iterative algorithms for solving the monotone bilevel equilibrium problem (MBEP) with the GSVI and CFPP constraints. Some strong convergence results for the proposed algorithms are established under the mild assumptions.

## [03072] New strong convergence theorems of generalized quasi-contractive mappings

**Author(s)** : Yangqing Qiu (Shanghai Polytechnic University)

**Abstract** : In this paper, the strong convergences and estimates of convergence rate for generalized quasi-contractive mappings and generalized set-valued quasi-contractive mappings are studied in a real Hilbert space. Firstly, the Picard iterative process is used to approximate the fixed point. Secondly, a characterization of strong convergence theorem of the Mann iterative sequence is proved. By virtue of the mean value theorem of integrals, the convergence rate and the error estimate of the iterative processes are given.

02404 (2/4) : 1D @E606

## [03144] Mittag-leffler stability of Fractional-order Neural Networks with time-varying delays

**Author(s)** : wei ding xiang zhu (Shanghai Normal University)

**Abstract** : This paper mainly studies a kind of fractional-order neural networks with time-varying delays. By using the mean value theorem of integrals, inequality technique and Banach fixed point theorem, the Mittag-leffler stability of the unique equilibrium point of the system can be proved when some satisfied conditions are built.

## [03170] Singular Riemann problems and their applications

**Author(s)** : Aifang Qu (Shanghai Normal University)

**Abstract** : In this talk, we will focus on a class of singular Riemann problems which contain concentration supported at the initial discontinuity. It corresponds to the study of a class of measure partial differential equations. Further, we will briefly introduce some applications of these problems to the study of hypersonic limit flow passing a wedge, fluid-structure interaction problems and conservation laws with discontinuous flux.

## [03270] Gas-liquid Phase Transition Problem for Non-isentropic Compressible Euler Equations

**Author(s)** : Pei-yu Zhang (Shanghai Normal University)

**Abstract** : We study gas-liquid phase transition problem described by one-dimensional non-isentropic Euler equations. For this purpose, we solve the Riemann problem for non-isentropic Euler equations in the class of Radon measure. The difficulty is to find a meaningful solution to Riemann problem that satisfies the occurrence of this gas-liquid phase transformation phenomenon. This provide a new way of thinking for the study of gas-liquid phase transition.

## [03286] Accelerated subgradient-extragradient methods for VIPs and CFPPs implicating countable nonexpansive-operators

**Author(s)** : Yun-ling Cui (shanghai normal university)

**Abstract** : In a real Hilbert space, let the VIP and CFPP denote the variational inequality problem and common fixed-point problem of countable nonexpansive operators and asymptotically nonexpansive operator, respectively. In this paper, we construct two modified Mann-type subgradient extragradient rules with a linear-search process for finding a common solution of the VIP and CFPP. We demonstrate the strong convergence of the suggested rules to a common solution of the VIP and CFPP.

02404 (3/4) : 1E @E606

## [03591] The Behaviors of Rupture Solutions for a Class of Elliptic MEMS Equations

**Author(s)** : Yanyan Zhang (East China Normal University)

**Abstract** : We will talk about the rupture solutions of a semilinear elliptic equation

$$\Delta u = \frac{\lambda|x|^\alpha}{u^p}, \quad x \in \mathbb{R}^2 \setminus \{0\}, u(0) = 0, \lambda > 0, p > 0, \alpha > -2,$$

which derived from fields such as Micro-Electro-Mechanical System(MEMS). The remarkable feature of MEMS equations is the singularity of nonlinear terms.

In this talk, we will firstly analysis the classification of all possible singularities at  $x = 0$  for rupture solutions  $u(x)$ . In particular, we show that for some  $(\alpha, p)$ ,  $u(x)$  admits only the isotropic singularity at  $x = 0$ , and otherwise  $u(x)$  may admit the anisotropic singularity at  $x = 0$ . Secondly, global solutions in  $\mathbb{R}^2 \setminus \{0\}$ (their existence and their behavior near  $x = \infty$  as well as near  $x = 0$ ) are also studied.

These results contribute to providing theoretical basis for the design and application of MEMS devices.

This is a joint work with Y.J. Guo, F. Zhou and Qing Li.

02404 (4/4) : 2C @E606

## [02406] European Research Council (ERC) information session

**Session Time & Room :** 3E (Aug.23, 17:40-19:20) @G301

**Type :** Proposal of Minisymposium

**Abstract :** The European Research Council is the premier European funding organisation for excellent frontier research. Its mission is to encourage highest quality research in Europe through competitive funding and to support investigator-driven frontier research across all fields, based on scientific excellence.

In this minisymposium, ERC laureates will present their work in various grant schemes. The ERC office in Brussels will present the main opportunities for researchers. The final talk will concentrate on how to build a specific grant office within a university mathematics department, to stimulate researchers to apply for many different types of grants, including those of the ERC.

**Organizer(s) :** Alfio Quarteroni, Wil Schilders

**Classification :** 00A05

**Minisymposium Program :**

02406 (1/1) : 3E @G301 [Chair: Wil Schilders and Alfio Quarteroni]

## [03125] European Research Council (ERC): insight into funding opportunities

**Format :** Talk at Waseda University

**Author(s) :** Joan Vazquez Molina (European Research Council Executive Agency)

**Abstract :** The ERC's mission is to encourage the highest quality research in Europe through competitive funding and to support investigator-driven frontier research across all fields, based on scientific excellence. I will give an overview of our funding opportunities, which are open to researchers from any nationality and at any career stage. I will provide insight into our evaluation and selection process, focusing on details of particular interest for the industrial and applied mathematics community.

## [05538] Building a new mathematical adventure with ERC support.

**Author(s) :** Alfio Quarteroni (Politecnico di Milano)

**Abstract :** The generous ERC support has enabled me to lay the scientific foundations for computational medicine, an immensely captivating field that presents extraordinary mathematical challenges while offering the opportunity to contribute to solving complex problems of clinical and societal significance. In this presentation, I will outline the key milestones of this journey, and briefly touch upon my decade-long experience as the chairman of the ERC Mathematical Panel for Consolidator Grants.

## [05548] Extreme-scale Mathematically-based Computational Chemistry Synergy project

**Author(s) :** Laura Grigori (EPFL and PSI)

**Abstract :** In this talk we will describe the ERC Synergy project entitled Extreme-scale Mathematically-based Computational Chemistry. Molecular simulation is one of the most dynamic areas of scientific computing. Its field of application is very broad, ranging from theoretical chemistry and drug design to materials science and

nanotechnology. We will review in this talk some of the research topics, challenges and achievements of this multidisciplinary effort that was made possible by ERC-Synergy-type funding.

## [05567] A dedicated Project Development Office for Mathematics

**Author(s)** : Wil Schilders (Eindhoven University of Technology)

**Abstract** : At Eindhoven University, end of 2013 we started a Project Development Office (PDO) within the Department of Mathematics and Computer Science. This office has all the knowledge and expertise to inform mathematicians about suitable project opportunities, disregarding less suitable options, and helps actively with the writing of proposals. Personal grants like ERC proposals are of prime importance, PDO has a database of successful proposals. It has turned out to be a very successful move, other university departments and universities are copying the concept.

## [02408] Recent advances in two-phase flow influenced by thermal fluctuations

**Session Time & Room :**

02408 (1/3) : 5B (Aug.25, 10:40-12:20) @F412

02408 (2/3) : 5C (Aug.25, 13:20-15:00) @F412

02408 (3/3) : 5D (Aug.25, 15:30-17:10) @F412

**Type** : Proposal of Minisymposium

**Abstract** : Thermal fluctuations may influence the evolution of interfaces in multi-phase flow. For this reason, analysis and numerics of stochastic versions of Allen-Cahn or Cahn-Hilliard equations with multiplicative noise, sometimes coupled to momentum equations of fluid dynamics, gained the interest of researchers both in pde and in stochastics. Related to these questions is the investigation of stochastic thin-film equations with their fascinating interplay between degenerate parabolicity and multiplicative noise.

This mini-symposium is supposed to bring researchers together who recently made important contributions both to analysis and numerics of such problems and to foster new collaborations.

**Organizer(s)** : Günther Grün, Stefan Metzger

**Classification** : 60H15, 35Q35, 76A20, 76T10

**Minisymposium Program :**

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02408 (1/3) : 5B @F412 [Chair: Stefan Metzger]

## [03080] The stochastic Navier-Stokes-Allen-Cahn system with singular potential

**Format** : Talk at Waseda University

**Author(s)** : Andrea Di Primio (Politecnico di Milano)Maurizio Grasselli (Politecnico di Milano)Luca Scarpa (Politecnico di Milano)

**Abstract** : In this talk, I consider the stochastic Navier-Stokes-Allen-Cahn system in a bounded domain of  $\mathbb{R}^d$ , with  $d \in \{2, 3\}$ , and give some insights on the existence of martingale (in two and three dimensions) and probabilistically-strong solutions (in two dimensions). With respect to its deterministic counterpart, two independent cylindrical stochastic perturbations, which account for thermodynamical effects (e.g., microscopic collisions), are introduced. Moreover, a singular potential is considered, as prescribed by the thermodynamical derivation of the model.

## [03081] On some stochastic phase-field models of Cahn-Hilliard-Cook type with logarithmic potential

**Format** : Online Talk on Zoom

**Author(s)** : Luca Scarpa (Politecnico di Milano)

**Abstract** : We give an overview of some recent results on stochastic phase-field models with logarithmic potential, which cover the celebrated Cahn-Hilliard-Cook equation. Both the conservative and the non-conservative cases are considered, as well as degenerate and non-degenerate mobilities. Well-posedness, regularity, and long-time

part\_2

behaviour of solutions are discussed, with a mention on uniqueness-by-noise. The works presented in the talk are based on joint collaborations with A. Di Primio, Prof. M. Grasselli, and Dr. M. Zanella.

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02408 (2/3) : 5C @F412 [Chair: Max Sauerbrey]

### [03044] Temperature Effects in Generalized Diffusions

**Format :** Talk at Waseda University

**Author(s) :** Chun Liu (Illinois Tech)

**Abstract :** Abstract: In this work, we will introduce a general framework to derive thermodynamics of a mechanical system, which guarantee the consistence between the energetic variational approaches with the laws of thermodynamics. In particular, we will focus on the coupling between the thermal and mechanical forces. We will also present some analysis results and difficulties to these systems.

### [04783] Asymptotics of the stochastic Cahn-Hilliard equation with space-time white noise

**Format :** Online Talk on Zoom

**Author(s) :** Lubomir Banas (Bielefeld University)

**Abstract :** We study the sharp interface limit of the stochastic Cahn-Hilliard equation with space-time white noise. We show that for sufficiently strong scaling of the noise the solution of the equation converges to the solution of the deterministic Hele-Shaw problem. We also discuss corresponding results for the numerical approximation of the problem.

### [03980] Weak error analysis for the stochastic Allen-Cahn equation

**Format :** Online Talk on Zoom

**Author(s) :** Dominic Breit (TU Clausthal)Andreas Prohl Tuebingen (University of Tuebingen)

**Abstract :** We prove strong rate  $\{\backslash em resp.\} \sim$  weak rate  $\mathcal{O}(\tau)$  for a structure preserving temporal discretization (with  $\tau$  the step size) of the stochastic Allen-Cahn equation with additive  $\{\backslash em resp.\} \sim$  multiplicative colored noise in  $d = 1, 2, 3$  dimensions.

Direct variational arguments exploit the one-sided Lipschitz property of the cubic nonlinearity in the first setting to settle first order strong rate. It is the same property which allows for uniform bounds for the derivatives of the solution of the related Kolmogorov equation, and then leads to weak rate  $\mathcal{O}(\tau)$  in the presence of multiplicative noise. Hence, we obtain twice the rate of convergence known for the strong error in the presence of multiplicative noise.

### [03932] On a convergent SAV scheme for stochastic phase-field equations

**Format :** Talk at Waseda University

**Author(s) :** Stefan Metzger (FAU Erlangen-Nürnberg)

**Abstract :** In this talk, we discuss the numerical treatment of stochastic Cahn-Hilliard equations with stochastic dynamic boundary conditions. These equations can be used to describe contact line tension effects in two-phase flows. By applying a stochastic version of the SAV method, we derive a stable, fully discrete finite element scheme that is linear with respect to the unknown quantities. Furthermore, we establish convergence of the discrete solutions towards martingale solutions using Skorokhod-type arguments.

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02408 (3/3) : 5D @F412 [Chair: Stefan Metzger]

### [03355] Martingale solutions to the stochastic thin-film equation in two dimensions

**Format :** Talk at Waseda University

**Author(s) :** Max Sauerbrey (TU Delft)

**Abstract :** We construct solutions to the stochastic thin-film equation with quadratic mobility and Stratonovich gradient noise in the physically relevant dimension  $d = 2$  and allow in particular for solutions with non-full support. The construction relies on a Trotter-Kato time-splitting scheme, which was recently employed in  $d = 1$ .

The additional analytical challenges due to the higher spatial dimension are overcome using  $\alpha$ -entropy estimates and corresponding tightness arguments.

## [04416] SOLUTIONS TO THE STOCHASTIC THIN-FILM EQUATION FOR INITIAL VALUES WITH NON-FULL SUPPORT

**Format :** Online Talk on Zoom

**Author(s) :** Manuel Victor Gnann (Delft University of Technology)Konstantinos Dareiotis (University of Leeds)Benjamin Gess (Bielefeld University and Max Planck Institute for Mathematics in the Sciences, Leipzig)Günther Grün (University of Erlangen-Nuremberg)Max Sauerbrey (TU Delft)

**Abstract :** We prove existence of non-negative martingale solutions to a class of stochastic degenerate-parabolic fourth-order PDEs arising in surface-tension driven thin-film flow influenced by thermal noise. The construction applies to a range of mobilities including the cubic one which occurs under the assumption of a no-slip condition at the liquid-solid interface. Since their introduction more than 15 years ago, by Davidovitch, Moro, and Stone, and by Gruen, Mecke, and Rauscher, the existence of solutions to stochastic thin-film equations for cubic mobilities has been an open problem, even in the case of sufficiently regular noise. Our proof of global-in-time solutions relies on a careful combination of entropy and energy estimates in conjunction with a tailor-made approximation procedure to control the formation of shocks caused by the nonlinear stochastic scalar conservation law structure of the noise. The construction of solutions with non-full support for the initial data using alpha-entropies shall be discussed.

## [04240] Existence of positive solutions to stochastic thin-film equations in the case of weak slippage

**Format :** Talk at Waseda University

**Author(s) :** Lorenz Klein (FAU Erlangen-Nürnberg)Günther Grün (FAU Erlangen-Nürnberg)

**Abstract :** We study stochastic thin-film equations for flow governed by surface tension and conjoining/disjoining interface potentials. For mobility exponents  $n \in (2, 3)$ , we construct martingale solutions via spatial discretization, energy-entropy estimates based on stopping time arguments, and stochastic compactness methods. A crucial ingredient to extend methods used in the case  $n = 2$  are new discrete formulas for integration by parts which allow to treat nonlinearities related to Stratonovich correction terms.

This is joint work with G. Grün.

## [04442] On finite speed of propagation for stochastic thin-film equations

**Format :** Online Talk on Zoom

**Author(s) :** Günther Grün (FAU Erlangen-Nürnberg)Lorenz Klein (FAU Erlangen-Nürnberg)

**Abstract :** In this talk, we present an energy method which allows to prove finite speed of propagation for sufficiently regular solutions to a class of stochastic thin-film equations with conservative multiplicative noise under periodic boundary conditions. Analytically, our approach is based on novel integral estimates combined with appropriate modifications of the technique previously used for stochastic porous-media and stochastic parabolic  $p$ -Laplace equations.

# [02411] Recent Advances in Numerical Methods for Nonlinear Equations and Applications

**Session Time & Room :**

02411 (1/3) : 4C (Aug.24, 13:20-15:00) @E604

02411 (2/3) : 4D (Aug.24, 15:30-17:10) @E604

02411 (3/3) : 4E (Aug.24, 17:40-19:20) @E604

**Type :** Proposal of Minisymposium

**Abstract :** Nonlinear equations and systems of equations are commonly used to describe scientific and engineering challenges. There are more and more applications for these systems, and majority of the techniques, now in use, have limitations and drawbacks. Thus, it is crucial to create novel numerical techniques that are part\_2

exceptionally accurate, stable, and reliable. This symposium focuses on the contemporary design methodologies, including machine learning algorithms, conformable fractional equations, and others, to real-world problems such as metabolic pathways, drug delivery interaction problem, image segmentation etc. We bring researchers from a broad spectrum to discuss development and applications of these modern methods.

**Organizer(s)** : Fiza Zafar, Alicia Cordero, Juan Ramon Torregrosa and Norma Binti Alias

**Classification** : 65H05, 65H10, 65Y05, 65Y10, 65B99

**Minisymposium Program :**

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02411 (1/3) : 4C @E604 [Chair: Fiza Zafar]

### [03387] Efficient iterative scheme for system of nonlinear equations

**Format** : Online Talk on Zoom

**Author(s)** : Himani Arora (Guru Nanak Dev University, Amritsar)

**Abstract** : Solving systems of nonlinear equations is an important and interesting task in science and engineering. But finding a solution of these systems using analytical methods is almost impossible, so one has to rely on iterative techniques for solution of such problems. The main motive of this talk is to discuss an efficient iterative technique for solving systems of nonlinear equations. The most time consuming and hard task while designing an iterative scheme is the evaluation of the inverse of the derivative. The main feature of the scheme presented is that it only utilizes one inverse evaluation per iteration, which makes the scheme computationally efficient. The efficiency of the scheme is verified through a number of real-world problems like integral equations and boundary value problems etc.

### [03084] Non-Linear GAC Model for GIS Image Segmentation of Deforestation in Nusajaya Malaysia

**Format** : Online Talk on Zoom

**Author(s)** : norma binti alias (universiti teknologi malaysia)fiza zafar (Bahauddin Zakariya University)

**Abstract** : Based on the statistical data from website Global Forest Watch, from year 2001 to 2021, Nusajaya , Johor Malaysia experience a loss of 745kha of tree cover which is equivalent to a 47% decrease and a 292Mt of increase in CO<sub>2</sub> emissions . GIS images able to visualize the deforestation problem. Digital transformation of images can be analysed by non-linear GAC Model for image segmentation. Numerical performance evaluation obtained the validation and verification of the analysis.

### [03352] Analysis of Love-type wave in a nonlocal piezoelectric composite

**Format** : Talk at Waseda University

**Author(s)** : Vanita Sharma (SVKM's NMIMS Chandigarh)

**Abstract** : The aim of this research article is to provide a more detailed investigation of the size influences in piezoelectric material subjected to Love-type wave propagation. With the goal to consider the size influences of the structure, the Eringen's nonlocal theory is utilized. The dispersion relations for piezoelectric composite are obtained. Thereafter, detailed investigations of various affecting parameters viz. nonlocal parameter, material parameters etc. on the wave dispersion characteristics of size-dependent nanoscaled structure are addressed.

### [03396] Mathematical modelling of Wave Equation in Elastodynamics Problems

**Format** : Online Talk on Zoom

**Author(s)** : Maryam Abdullah Alharbi (UTM)Norma binti Alias (UTM)

**Abstract** : The study of the wave equation in elastodynamics is crucial for understanding various physical phenomena. We present a mathematical model that describes the behavior of waves in elastodynamics. The model is stable to solve using FDM, which means this model is convergent to the approximate solution. Additionally, we highlight the relationship between blood flow and elastodynamics. We discuss the behavior of blood vessels and their interaction with blood as a fluid.

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02411 (2/3) : 4D @E604 [Chair: Alicia Cordero]

## [03928] Iterative Newton type methods with fractional derivatives

**Format :** Online Talk on Zoom

**Author(s) :** Juan R. Torregrosa (Universitat Politècnica de València)Alicia Cordero (Universitat Politècnica de València)Paula Triguero Navarro (Universitat Politècnica de València)

**Abstract :** Recently, several iterative methods using fractional derivatives have been designed. In this work, we propose some iterative schemes with fractal and conformable derivatives for solving nonlinear equations  $f(x) = 0$ . We analyze the local convergence of these algorithms and study their stability and computational performance. This stability is compared with those of iterative procedures using standard derivatives.

## [03702] A Hybrid Genetic Algorithm for Solving Nonlinear Systems and Applications

**Format :** Talk at Waseda University

**Author(s) :** Fiza Zafar (CASPAM, Bahauddin Zakariya University, Pakistan)Nabeera Ahmad Gillani (CASPAM, Bahauddin Zakariya University, Pakistan)

**Abstract :** In this talk, a hybrid genetic algorithm has been proposed to solve nonlinear systems of equations by combining genetic algorithm and a fourth order convergent Jarratt type method to guarantee convergence and to accelerate the process of obtaining the solution. The proposed method is then applied to optimize biochemical systems to maximize the production and minimize the reaction's concentration. The performance and computational time of genetic algorithm and hybrid genetic algorithm have also been analyzed.

## [03357] Iterative Method for Efficiently Computing Generalized Inverses of Matrices

**Format :** Talk at Waseda University

**Author(s) :** MANPREET KAUR (Lovely Professional University)

**Abstract :** The study of generalized inverses of matrices has been extensively explored in recent years. An iterative approach for finding the Moore-Penrose inverse of a matrix is discussed. The method's convergence is analyzed, achieving fourth-order convergence under certain conditions, with a suggested parameter choice for improved convergence order. Testing on real-life matrices from the Matrix-Market Library shows the proposed scheme's superiority over existing methods. The study also investigates the most efficient parameter choice.

## [03376] Globally convergent iterative method for evaluating matrix sign function

**Format :** Talk at Waseda University

**Author(s) :** Munish Kansal (Thapar Institute of Engineering and Technology, Patiala, Punjab 147004)

**Abstract :** The matrix sign function plays a vital role in the various fields of scientific computing. This work proposes an iterative method to compute the matrix sign function of a matrix having no eigenvalues on the imaginary axis and is analyzed for convergence and asymptotic stability. Global convergence behavior is provided by drawing basins of attraction. Numerical experiments of different dimensions support the theoretical results and illustrate the efficiency of the proposed method.

02411 (3/3) : 4E @E604 [Chair: Juan Ramon Torregrosa]

## [03040] An Iterative scheme for finding simultaneous roots of nonlinear systems

**Format :** Talk at Waseda University

**Author(s) :** Neus Garrido (Universitat Politècnica de València)Paula Triguero Navarro (Universitat Politècnica de València)Alicia Cordero (Universitat Politècnica de València)Juan Ramón Torregrosa (Universitat Politècnica de València)

**Abstract :** Systems of nonlinear equations usually appear in many real-world applications. We give a general iterative algorithm to approximate simultaneous solutions of systems of nonlinear equations. We show that by adding a general sub-step to any iterative method, a new iterative scheme to approximate simultaneous roots of nonlinear systems with doubled convergence order can be obtained. We add this sub-step to some iterative methods of this domain and analyze the behavior of the new schemes.

## [03925] High-order iterative methods for solving nonlinear systems

**Format :** Online Talk on Zoom

**Author(s) :** Alicia Cordero Renso V. Rojas-Hiciano (Pontificia Universidad Católica Madre y Maestra) Juan R. Torregrosa (Universitat Politècnica de València)

**Abstract :** In the last decades, many optimal iterative schemes have been developed for solving nonlinear equations, for simple or multiple roots. However, the amount of vectorial iterative procedures able to estimate the solutions of nonlinear systems could be higher. The computational cost of solving the linear systems involved in each iteration plays a key role in the design, seeking the efficiency of the method. We present a highly efficient scheme for solving nonlinear systems of equations.

## [02423] Non-standard finite element methods

**Session Time & Room :**

02423 (1/2) : 2C (Aug.22, 13:20-15:00) @E711

02423 (2/2) : 2D (Aug.22, 15:30-17:10) @E711

**Type :** Proposal of Minisymposium

**Abstract :** This minisymposium is on the non-standard finite element methods, including mixed finite element methods, non-conforming finite elements methods, discontinuous Galerkin methods, virtual element methods, weak Galerkin methods, and so on. This minisymposium intended to focus on the latest research progress in the field of numerical methods of partial differential equations. It is expected that through the frontier progress report, scholars engaged in the research of numerical methods of partial differential equations can be exposed to the core problems in the field of mathematical theory, numerical methods, and practical applications.

**Organizer(s) :** Carsten Carstensen, Jun Hu, Ran Zhang

**Classification :** 65N30, 65M60, 65N25

**Minisymposium Program :**

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02423 (1/2) : 2C @E711 [Chair: Jun Hu]

## [04214] A posteriori error estimation for a C<sup>1</sup>-virtual element method of Kirchhoff plates

**Author(s) :** Jianguo Huang (Shanghai Jiao Tong University)

**Abstract :** A residual-type a posteriori error estimation is developed for a  $C^1$ -conforming virtual element method (VEM) to solve a Kirchhoff plate bending problem. As an outcome of the error estimator, an adaptive VEM is introduced using the mesh refinement strategy with the one-hanging-node rule. A series of numerical results are performed to verify the efficiency of the method. This is a joint work with Mingqing Chen and Sen Lin from Shanghai Jiao Tong University.

## [03654] Stabilization-Free Virtual Element Methods

**Author(s) :** Xuehai Huang (Shanghai University of Finance and Economics)

**Abstract :** Stabilization-free virtual element methods (VEMs) in arbitrary degree of polynomial are developed for second order elliptic problems, including a nonconforming VEM in arbitrary dimension and a conforming VEM in two dimensions. The key is to construct local  $H(\div)$ -conforming macro finite element spaces such that the associated  $L^2$  projection of the gradient of virtual element functions is computable, and the  $L^2$  projector has a uniform lower bound on the gradient of virtual element function spaces in  $L^2$  norm. Optimal error estimates are derived for these stabilization-free VEMs. Numerical experiments are provided to test the stabilization-free VEMs.

## [03806] Discontinuous Galerkin methods for magnetic advection-diffusion problems

**Author(s)** : Jindong Wang (Peking University) Shuonan Wu (Peking University)

**Abstract** : We devise and analyze a class of the primal discontinuous Galerkin methods for magnetic advection-diffusion problems based on the weighted-residual approach. In addition to the upwind stabilization, we find a new mechanism under the vector case that provides more flexibility in constructing the schemes. For the more general Friedrichs system, we show the stability and optimal error estimate, which boil down to two core ingredients -- the weight function and the special projection -- that contain information of advection. Numerical experiments are provided to verify the theoretical results.

## [03492] Some finite element divdiv complexes in three dimensions

**Format** : Talk at Waseda University

**Author(s)** : Rui Ma (Beijing Institute of Technology)

**Abstract** : This talk will present two families of finite element divdiv complexes on tetrahedral grids and one family on cuboid grids. They can be used to discretize the linearized Einstein-Bianchi system.

02423 (2/2) : 2D @E711 [Chair: Ran Zhang]

## [04728] Adaptive FEM for Helmholtz equation with large wave number

**Author(s)** : Haijun Wu (Nanjing University) Songyao Duan (Nanjing University)

**Abstract** : A posteriori upper and lower bounds are derived for the finite element method (FEM) for the Helmholtz equation with large wavenumber. It is proved rigorously that the standard residual type error estimator seriously underestimates the true error of the FE solution for the mesh size  $h$  in the preasymptotic regime, which is first observed by [Babuska,~et-al., A posteriori error estimation for finite element solutions of Helmholtz equation. Part I, Int. J. Numer. Meth. Engrg. 40, 3443--3462 (1997)] for a one dimensional problem. By establishing an equivalence relationship between the error estimators for the FE solution and the corresponding elliptic projection of the exact solution, an adaptive algorithm is proposed and its convergence and quasi-optimality are proved under the condition that  $k^{2p+1}h_0^{2p}$  is sufficiently small, where  $k$  is the wavenumber,  $h_0$  is the initial mesh size.

## [03581] Stable Finite Element Scheme for Dynamic Ginzburg-Landau Equations

**Author(s)** : Limin Ma (Wuhan University)

**Abstract** : We propose a decoupled numerical scheme of the time-dependent Ginzburg-Landau equations under the temporal gauge. The maximum bound principle of the order parameter and the energy dissipation law in the discrete sense are proved, which can guarantee the stability and validity of the numerical simulations, and further facilitate the adoption of adaptive time-stepping strategy. An optimal error estimate of the proposed scheme is also proved and verified by numerical examples.

## [03508] Local bounded commuting projection operators for discrete finite element complexes

**Author(s)** : Ting Lin (Peking University)

**Abstract** : Local bounded commuting projection operators are an important tool in the analysis of finite element exterior and mixed finite element methods. However, so far only those of the standard finite element spaces have been discussed. In this talk, I will introduce the construction of local bounded commuting projection operators of the discrete finite element complexes, with some possible applications. The techniques developed here also give us a new perspective on the construction of finite element complexes.

## [04168] The weak Galerkin method for elliptic eigenvalue problems

**Author(s)** : Qilong Zhai (Jilin University)

**Abstract** : In this report, we propose and analyze the elliptic eigenvalue problems by using the weak Galerkin method. In contrast to the conforming finite element method, the lower bounds of eigenvalues are considered. We prove that the weak Galerkin method produces asymptotic lower bounds by using the high order polynomials, and produces guaranteed lower bounds by using the lowest order polynomials. Some numerical acceleration

techniques are also applied to the weak Galerkin method, and the numerical experiments are presented to verify the theoretical analysis.

## [02426] Mathematics of turbulent transport and coherent structures

### **Session Time & Room :**

02426 (1/2) : 5B (Aug.25, 10:40-12:20) @D401

02426 (2/2) : 5C (Aug.25, 13:20-15:00) @D401

### **Type :** Proposal of Minisymposium

**Abstract :** The transport of momentum and heat by coherent structures in turbulence has long been a central concern in fluid mechanics, especially because of its critical importance in industry, geophysics, and astrophysics. Significant progress has been made in recent years in Navier-Stokes-based variational principles, asymptotic analysis, and dynamical systems theory, finally producing meaningful results for practical applications. This minisymposium aims to bring together experts with a wide range of related backgrounds, from applied to fundamental, to exchange the latest findings and to set new research directions.

**Organizer(s) :** Kengo Deguchi; Shingo Motoki

**Classification :** 76F25, 76F20, 35A15, 35C20

### **Minisymposium Program :**

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02426 (1/2) : 5B @D401 [Chair: Shingo Motoki]

## [04104] Analysis of transport by coherent structures; overview

### **Format :** Talk at Waseda University

**Author(s) :** Kengo Deguchi (Monash University)

**Abstract :** A primary ongoing problem in fluid mechanics is the need to comprehend the large-scale average transport features of turbulent flows. For example, the prediction or improvement of heat/momentum transport is critical in a wide range of applications, but currently it relies on trial and error with massive amounts of experiments/simulations. A natural question arises: can we explain the mechanism of the transport logically based on Navier-Stokes equations? The key to the answer seems to lie in the coherent structures in turbulence, and an overview of recent developments will be given in the talk.

## [04490] Analysis, modeling, and simulation of slow-fast quasilinear dynamical systems

### **Format :** Online Talk on Zoom

**Author(s) :** Greg Chini (University of New Hampshire)

**Abstract :** We describe a new formalism for quasilinear systems exhibiting slow mean and fast, possibly unstable, linearized fluctuation dynamics. Using ODE and PDE models, we show that a slaving relation for the fluctuation amplitude can be derived by exploiting the tendency for the dynamics to self-organize on a slow marginal-stability manifold. Transient, fully nonlinear bursting events also can be predicted and systematically incorporated into our formalism. We conclude with an application to strongly stratified Kolmogorov flow.

## [04122] Steady coherent states in Rayleigh–Bénard convection

### **Format :** Online Talk on Zoom

**Author(s) :** Baole Wen (New York Institute of Technology)David Goluskin (University of Victoria)Gregory Chini (University of New Hampshire)Charles Doering (University of Michigan)

**Abstract :** A central question in Rayleigh–Bénard convection is how the Nusselt number  $Nu$  depends on the Rayleigh number  $Ra$  as  $Ra \rightarrow \infty$ . Experiments/simulations have yet to rule out either 'classical' 1/3 or 'ultimate' 1/2 asymptotic scaling. Here we show that certain steady rolls have classical 1/3 scaling and they transport more heat than turbulent experiments/simulations at comparable parameters. If turbulent heat transport continues to be dominated by steady transport asymptotically, it cannot achieve ultimate scaling.

## [04022] Optimal heat transport using branching flows

**Format :** Online Talk on Zoom

**Author(s) :** Anuj Kumar (University of California Santa Cruz)

**Abstract :** We are interested in the design of forcing in the Navier–Stokes equation such that the resultant flow maximizes the transport of a passive temperature between two differentially heated walls for a given power supply budget. Previous work established that the transport cannot scale faster than 1/3-power of the power supply. Recently, Doering & Tobasco (CPAM’19) constructed self-similar two-dimensional steady branching flows, saturating this upper bound up to a logarithmic correction to scaling. We present a construction of three-dimensional “branching pipe flows” that eliminates the possibility of this logarithmic correction and for which the corresponding passive scalar transport scales as a clean 1/3-power law in power supply. Our flows resemble previous numerical studies of the three-dimensional wall-to-wall problem by Motoki, Kawahara & Shimizu (J. Fluid Mech. vol.851, 2018, p.R4). However, using an unsteady branching flow construction, it appears that the 1/3 scaling is also optimal in two dimensions. After carefully examining these designs, we extract the underlying physical mechanism that makes the branching flows “efficient.”

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02426 (2/2) : 5C @D401 [Chair: Kengo Deguchi]

## [04552] Optimisation of horizontal periodicity in steady Rayleigh–Bénard convection

**Format :** Talk at Waseda University

**Author(s) :** Shingo Motoki (Osaka University)Genta Kawahara (Osaka University)Masaki Shimizu (Osaka University)

**Abstract :** Using a Newton–Krylov iteration, we have investigated steady solutions to the Boussinesq equations for Rayleigh–Bénard convection in a square periodic domain between horizontal walls with a constant temperature difference. We have found that a family of three-dimensional steady solutions with an optimal horizontal periodicity achieves higher wall-to-wall heat flux than those of two-dimensional solutions and turbulent states and exhibits the classical scaling commonly observed in convective turbulence.

## [04406] Chaos and unstable periodic orbits in subcritical Taylor-Couette flow

**Format :** Talk at Waseda University

**Author(s) :** Baoying Wang (Universitat Politècnica de Catalunya)Roger Ayats (Institute of Science and Technology Austria (ISTA))Kengo Deguchi (Monash University)Alvaro Meseguer (Universitat Politècnica de Catalunya)Fernando Mellibovsky (Universitat Politècnica de Catalunya)

**Abstract :** Although spectral approximation of turbulence typically requires a large number of modes, for relatively low Reynolds numbers the turbulent attractor lies on a low-dimensional manifold in phase space. The most extreme case is when the main features of the chaotic attractor can be quantified by a one-dimensional map on Poincaré section. We find this can indeed happen in subcritical Taylor-Couette flow, which should offer an important test case for connecting turbulence and periodic orbit analysis.

## [03988] The state-space structure of wall turbulence at high Reynolds numbers: a reduced-order model perspective

**Format :** Talk at Waseda University

**Author(s) :** Matthew McCormack (University of Edinburgh)André V. G. Cavalieri (Instituto Tecnológico de Aeronáutica)Yongyun Hwang (Imperial College London)

**Abstract :** Invariant solutions to the Navier-Stokes equations have been viewed to form the state-space skeleton of turbulence at low Reynolds numbers. However, as Reynolds number is increased, most of these invariant solutions currently computable were recently shown to be able to depict only partial processes of turbulence, and they neither resemble full-scale turbulence statistically nor dynamically. In this talk, I will present our recent efforts to understand the state-space structure of turbulence at moderately high Reynolds numbers in terms of invariant solutions utilising a reliable and robust reduced-order model.

## [03140] Coherent structures and the direct cascade in two-dimensional turbulence

**Format :** Talk at Waseda University

**Author(s) :** Roman O Grigoriev (Georgia Institute of Technology) Mateo Reynoso (Georgia Institute of Technology) Dmitriy Zhigunov (Georgia Institute of Technology)

**Abstract :** We describe a mechanism of the direct cascade in 2D turbulence which explains when the predictions of the classical Kraichnan-Leith-Batchelor theory hold, when deviations are found, and what causes these deviations. Coherent structures of two types play a key role in our theory: the first type describes the dynamics of the largest scales accessible to the flow, while the second type describes the dynamics of small-scale filamentary vorticity stretched and folded by the large-scale flow.

## [02435] Scaling Limits of Interacting Particle Systems

**Session Time & Room :**

02435 (1/3) : 4C (Aug.24, 13:20-15:00) @E501

02435 (2/3) : 4D (Aug.24, 15:30-17:10) @E501

02435 (3/3) : 4E (Aug.24, 17:40-19:20) @E501

**Type :** Proposal of Minisymposium

**Abstract :** This minisymposium aims to bring together young researchers in PDEs, probability and applied mathematics to share recent progress and complementary perspectives in the growing field of interacting particle systems. Such systems are not only important models in physics, biology, and many applied sciences, but also rich in mathematical structure.

Our topics include mean-field limits and propagation of chaos for large systems with singular interactions, limit theorems and large deviations for interacting particle systems on random graphs, particle and numerical methods of McKean-Vlasov PDEs, convergence theorems of SPDEs, and quasi-stationary behavior of SPDEs and their dual particle systems.

**Organizer(s) :** Wai-Tong (Louis) Fan, Zhenfu Wang, Ruoyu Wu

**Classification :** 60K35, 60F05, 35K55, 35Q49, 35Q70, interacting particle systems, mean-field limit, limit theorems of stochastic processes

**Minisymposium Program :**

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02435 (1/3) : 4C @E501 [Chair: Zhenfu Wang]

## [05450] Ergodic properties of rank-based diffusions

**Format :** Online Talk on Zoom

**Author(s) :** Sayan Banerjee (University of North Carolina, Chapel Hill) Amarjit Budhiraja (University of North Carolina, Chapel Hill)

**Abstract :** We investigate the long-time behavior of rank-based diffusions with infinitely many particles where the drift and diffusivity of each particle depends on its relative rank in the system. Unlike their finite dimensional analogues, such systems have infinitely many stationary measures and domains of attraction and extremality properties of such measures have been long-standing open questions. In this talk, we will explore some of these questions and provide answers to them in certain cases.

Based on joint works with Amarjit Budhiraja.

## [04342] Systems with Riesz Interactions in the Mean-Field Regime

**Format :** Online Talk on Zoom

**Author(s) :** Matthew Rosenzweig (MIT) Sylvia Serfaty (Courant Institute, NYU) Antonin Chodron de Courcel (Ecole Polytechnique)

**Abstract :** We present recent results on the large particle number and large time effective behavior of conservative or gradient dynamics for particle systems with mean-field interactions governed by a Coulomb or more general part\_2

Riesz potential and subject to possible noise modeling thermal fluctuations. The talk will discuss modulated energy/free energy techniques for studying the rate of mean-field convergence, how the rate deteriorates with time, and how fluctuations around the mean-field limit behave.

## [03026] Large Deviations for Multiscale Weakly Interacting Diffusions

**Format :** Online Talk on Zoom

**Author(s) :** Zachary Bezemek (Boston University)Konstantinos Spiliopoulos (Boston University)

**Abstract :** In this talk, we consider a collection of weakly interacting diffusion processes moving in a two-scale locally periodic environment. We study the large deviations principle of the empirical distribution of the particles' positions in the combined limit as the number of particles grow to infinity and the time-scale separation parameter goes to zero simultaneously. We derive several equivalent formulations of the rate function, making connections between a mean-field control formulation and the formulation of Dawson-Gärtner.

## [05239] Hydrodynamic Limits of non-Markovian Interacting Particle Systems on Sparse Graphs

**Format :** Online Talk on Zoom

**Author(s) :** Ankan Ganguly (University of Pennsylvania)Kavita Ramanan (Brown University)

**Abstract :** We consider hydrodynamic limits of non-Markovian interacting particle systems on large sparse graphs. Under mild conditions on the jump intensities and underlying graphs, it is shown that if the sequence of interaction graphs  $G_n$  converges locally in probability to a limit graph  $G$ , then the corresponding sequence of empirical measures of the particle trajectories converges weakly to the law of the marginal dynamics at the root vertex of  $G$ .

02435 (2/3) : 4D @E501 [Chair: Zhenfu Wang]

## [04551] Wave propagation for reaction-diffusion equations on infinite trees

**Format :** Online Talk on Zoom

**Author(s) :** Grigory Terlov (UNC Chapel Hill )Wai-Tong (Lous) Fan (Indiana University)Wenqing Hu (Missouri University of S&T)

**Abstract :** The asymptotic speed of the wavefront of the solution to FKPP equation on  $\mathbb{R}$  is well understood. I will present a probabilistic approach to the same problem on infinite metric trees. When the reaction rate is large enough we show that a travelling wavefront emerges. Its speed is slower than that of the same equation on the real line, and we can estimate this slow-down in terms of the structure of the tree.

## [03975] From the KPZ equation to the directed landscape

**Format :** Online Talk on Zoom

**Author(s) :** XUAN WU (University of Illinois Urbana-Champaign)

**Abstract :** This talk presents the convergence of the KPZ equation to the directed landscape, which is the central object in the KPZ universality class. This convergence result is the first to the directed landscape among the positive temperature models.

## [05115] Longtime behaviour of the stochastic FKPP equation conditioned on non-fixation

**Format :** Online Talk on Zoom

**Author(s) :** Oliver Kelsey Tough (University of Bath)Wai-Tong (Louis) Fan (Indiana University)

**Abstract :** In population genetics, fixation is the phenomenon in which all members of a population have the same copy of a given gene. Whilst most genes are fixed (most genes are shared by all individuals), not all genes are fixed (individuals aren't identical). The prototypical continuum model for the spread of a genetic type in a spatially distributed population under the effects of genetic drift, selection and migration is the stochastic Fisher-Kolmogorov-Petrovsky-Piscunov (FKPP) equation. We consider the stochastic FKPP equation on the circle. We establish existence and uniqueness of the quasi-stationary distribution (QSD) for solutions of the stochastic FKPP, considered to be absorbed upon fixation. We show that the distribution of the solution conditioned on non-fixation converges to this unique QSD as time  $t \rightarrow \infty$ , for any initial distribution. Moreover we characterise the leading-order asymptotics for the tail distribution of the fixation time. This is based on joint work with Wai-Tong Fan.

## [03336] The interacting multiplicative coalescent and Levy-like random fields

**Format :** Online Talk on Zoom

**Author(s) :** David J Clancy, Jr. (University of Wisconsin)

**Abstract :** The multiplicative coalescent describes the evolution of blocks where blocks of masses  $x$  and  $y$  form a single block of mass  $x + y$  at rate  $xy$ . This process naturally appears when studying many random graph models at criticality. Their marginal laws are described using (mixtures of) Levy-type processes. Using stochastic blockmodels, we show that one can describe the marginal law of two interacting multiplicative coalescences using a Levy-type random field. Based on work with V. Konarovskyi and V. Limic.

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02435 (3/3) : 4E @E501 [Chair: Zhenfu Wang]

## [03511] Graphon mean field systems

**Format :** Online Talk on Zoom

**Author(s) :** Ruoyu Wu (Iowa State University)Erhan Bayraktar (University of Michigan)Suman Chakraborty (Uppsala University)

**Abstract :** We consider heterogeneously interacting diffusive particle systems and their large population limit. The interaction is of mean field type with (random) weights characterized by an underlying graphon. The limit is given by a graphon particle system consisting of independent but heterogeneous nonlinear diffusions whose probability distributions are fully coupled. Well-posedness of the graphon particle system is established. A law of large numbers result is proved as the system size increases and the underlying graphons converge.

## [03358] Strong convergence of propagation of chaos for McKean-Vlasov SDEs with singular interactions

**Format :** Online Talk on Zoom

**Author(s) :** Zimo Hao (Bielefeld University)

**Abstract :** In this work we show the strong convergence of propagation of chaos for the particle approximation of McKean-Vlasov SDEs with singular  $L^p$ -interactions as well as for the moderate interaction particle systems on the level of particle trajectories. One of the main obstacles is to establish the strong well-posedness of the SDEs for particle systems with singular interaction. To this end, we extend the results on strong well-posedness of Krylov and R'ockner to the case of mixed  $L^p$ -drifts, where the heat kernel estimates play a crucial role. Moreover, when the interaction kernel is bounded measurable, we also obtain the optimal rate of strong convergence, which is partially based on Jabin and Wang's entropy method and Zvonkin's transformation.

## [03721] Nonlocal approximation of nonlinear diffusion equations

**Format :** Talk at Waseda University

**Author(s) :** José Antonio Carrillo (University of Oxford)Antonio Esposito (University of Oxford)Jeremy S.-H. Wu (UCLA)

**Abstract :** Nonlinear diffusion equations are ubiquitous in several real world applications. They were introduced to analyse gas expansion in a porous medium, groundwater infiltration, and heat conduction in plasmas, to name a few applications in physics. In this talk, I will present recent joint work with José A. Carrillo and Antonio Esposito concerning a nonlocal approximation inspired by the theory of gradient flows for a general family of equations closely related to the porous medium equation with  $m > 1$ . Our approximation is inspired by recent ideas to use (nonlocal) interaction equations to approximate (local) diffusion equations. We prove under very general assumptions that weak solutions to our nonlocal approximation converge to weak solutions of the original local equation. One byproduct of our analysis is the development of a deterministic particle method for numerically approximating solutions to nonlinear diffusion equations.

## [04156] Entropy-dissipation Informed Neural Network for McKean-Vlasov Type PDEs

**Format :** Online Talk on Zoom

**Author(s) :** Zebang Shen (ETH Zürich)Zhenfu Wang (Peking University)

**Abstract :** We extend the concept of self-consistency for the Fokker-Planck equation (FPE)(Shen et al., 2022) to the more general McKean-Vlasov equation (MVE). While FPE describes the macroscopic behavior of particles under drift and diffusion, MVE accounts for the additional inter-particle interactions, which are often highly singular in

physical systems. Two important examples considered in this paper are the MVE with Coulomb interactions and the vorticity formulation of the 2D Navier-Stokes equation. We show that a generalized self-consistency potential controls the KL-divergence between a hypothesis solution to the ground truth, through entropy dissipation. Built on this result, we propose to solve the MVEs by minimizing this potential function, while utilizing the neural networks for function approximation. We validate the empirical performance of our approach by comparing with state-of-the-art NN-based PDE solvers on several example problems.

## [02438] Recent advances in numerical multiscale methods

### **Session Time & Room :**

02438 (1/2) : 4D (Aug.24, 15:30-17:10) @E703

02438 (2/2) : 4E (Aug.24, 17:40-19:20) @E703

### **Type :** Proposal of Minisymposium

**Abstract :** Multiscale phenomena are ubiquitous in science and engineering, and many multiscale problems are modeled by partial differential equations with general rough coefficients. Direct numerical solution of such problems is often infeasible because a huge number of degrees of freedom are needed to resolve all details on all relevant scales. Numerical multiscale methods aim at reducing the computational cost by efficiently incorporating physically important fine-scale information into a coarse-grid representation. The scope of this minisymposium is to bring together experts in this field to present recent advances in the design and analysis of numerical multiscale methods.

**Organizer(s) :** Chupeng Ma, Robert Scheichl

**Classification :** 65M60, 65N15

### **Minisymposium Program :**

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02438 (1/2) : 4D @E703

## [03763] Super-Localized Generalized Finite Element Method

### **Format :** Talk at Waseda University

**Author(s) :** Moritz Hauck (University of Augsburg)Philip Freese (Technical University Hamburg)Tim Keil (University of Münster)Daniel Peterseim (University of Augsburg)

**Abstract :** We present a multi-scale method for elliptic PDEs with arbitrarily rough coefficients. The method constructs operator-adapted solution spaces with uniform algebraic approximation rates by combining techniques from numerical homogenization and partition of unity methods. Localized basis functions with the same super-exponential localization properties as the Super-Localized Orthogonal Decomposition (SLOD) allow for an efficient implementation of the method. We derive higher-order versions of the method and demonstrate its application to high-contrast channeled coefficients and Helmholtz problems.

## [03861] An efficient multiscale approach for simulating Bose-Einstein condensates

### **Format :** Talk at Waseda University

**Author(s) :** Christian Döding (Ruhr-University Bochum)Patrick Henning (Ruhr-University Bochum)Johan Wärnegård (Columbia University)

**Abstract :** In this talk we consider the numerical treatment of nonlinear Schrödinger equations as they appear in the modeling of Bose-Einstein condensates. We give numerical examples that demonstrate the influence of the discrete energy on the accuracy of numerical approximations and that a spurious energy can create artificial phenomena such as drifting particles. In order to conserve the exact energy of the equation as accurately as possible, we propose a combination of a class of conservative time integrators with a suitable multiscale finite element discretization in space. This space discretization is based on the technique of Localized Orthogonal Decompositions (LOD) and allows to capture general time invariants with a 6th order accuracy with respect to the chosen mesh size H. This accuracy is preserved due to the conservation properties of the time stepping method. The computational efficiency of the method is demonstrated for a numerical benchmark problem with known exact solution, which is however barely solvable with traditional methods on long time scales.

## [04037] Multigrid/multiscale solver for the radiative transfer equation in heterogeneous media

**Format :** Talk at Waseda University

**Author(s) :** QINCHEN SONG (Shanghai Jiao Tong University)

**Abstract :** The radiative transfer equation describes the interaction between particles and media such as gases, semitransparent liquids , solids, and porous materials, which is widely used in nuclear engineering, thermal radiation transport, etc. In the first part of our work, we construct a multigrid scheme for 1D neutron transport equation based on a second-order discretization scheme that is uniform with respect to  $\epsilon$  in the diffusion regime and valid up to the boundary layer and interface layer. We prove its multigrid convergence theoretically and justify it numerically. This multigrid scheme is special in a way that the smoothing procedure in the typical multigrid method can be skipped, which saves a large amount of computation. The 1D scheme can be adapted to the 2D case, and the resulting 2D scheme performs well in the diffusion regime. In the second part, we focus on the 2D radiative transport equation in the transport regime. After discretization of the equation, we get a sparse linear system of extremely high dimensions. Typically, we have 3 ways to solve the linear system: direct methods, iterative methods, and rank-structured methods, which requires computation cost of  $I^6$ ,  $I^3$  and  $I^3$  respectively (provided that the physical domain is discretized as a  $I \times I$  grid). In our work, we use a hybrid scheme of iterative methods and rank-structured methods and reduce the computation cost down to  $I^{5/2}$ . This is joint work with Min Tang (SJTU) and Lei Zhang (SJTU).

## [03533] EXPONENTIALLY CONVERGENT MULTISCALE METHODS FOR HIGH FREQUENCY HETEROGENEOUS HELMHOLTZ EQUATIONS

**Format :** Talk at Waseda University

**Author(s) :** Thomas Y Hou (California Institute of Technology)Yifan Chen (California Institute of Technology)Yixuan Wang (California Institute of Technology)

**Abstract :** We present a multiscale framework for solving the high frequency Helmholtz equation in heterogeneous media without scale separation. Our methods achieve a nearly exponential rate of convergence without suffering from the well-known pollution effect. The key idea is a coarse-fine scale decomposition of the solution space that adapts to the media property and wavenumber. The coarse part is of low complexity while the fine part is local such that it can be computed efficiently.

02438 (2/2) : 4E @E703

## [03853] A high-order method for elliptic multiscale problems

**Format :** Talk at Waseda University

**Author(s) :** Roland Maier (University of Jena)

**Abstract :** We present a multiscale approach for an elliptic multiscale setting with general unstructured diffusion coefficients that is able to achieve high-order convergence rates with respect to the mesh parameter and the polynomial degree. The method allows for suitable localization and does not rely on additional assumptions on the domain, the diffusion coefficient, or the exact (weak) solution as typically required for high-order approaches. Rigorous a priori error estimates with respect to the involved discretization parameters are presented and the interplay between these parameters as well as the performance of the method are studied numerically.

## [04038] Hierarchical Attention Neural Operator for Multiscale PDEs

**Format :** Talk at Waseda University

**Author(s) :** Bo Xu (Shanghai Jiao Tong University)

**Abstract :** Complex nonlinear interplays of multiple scales give rise to many interesting physical phenomena and pose significant difficulties for the computer simulation of multiscale PDE models in areas such as reservoir simulation, high-frequency scattering, and turbulence modeling. In this talk, we apply hierarchical attention to a data-driven operator learning problem related to multiscale partial differential equations. An empirical H1 loss function is proposed to counteract the spectral bias of the neural operator approximation for the multiscale solution space. We perform experiments on the multiscale Darcy Flow, Helmholtz equation and Navier-Stokes equation. Our model exhibits noticeably higher accuracy compared to the current neural operator techniques, and it produces state-of-the-art results across a variety of datasets. This is joint work with Xinliang Liu (KAUST) and Lei Zhang (SJTU).

## [04167] An abstract framework for multiscale spectral generalized FEMs

**Format :** Online Talk on Zoom

**Author(s) :** chupeng ma (Great Bay University)

**Abstract :** We present an abstract framework for multiscale spectral generalized FEMs based on locally optimal spectral approximations. A higher convergence rate for the local approximations than previously established is derived under certain conditions. The abstract theory is applied to various problems with strongly heterogeneous coefficients, including convection-diffusion problems, elasticity problems, high-frequency wave problems (Helmholtz, elastic wave, and Maxwell's equations), and fourth-order problems, both in the continuous and discrete settings.

## [03857] Multiscale multicontinuum problems in fractured porous media: dimension reduction and decoupling

**Format :** Talk at Waseda University

**Author(s) :** Maria Vasilyeva (Texas A&M University-Corpus Christi)

**Abstract :** We consider the coupled system of equations that describe flow in fractured porous media. To describe such types of problems, multicontinuum and multiscale approaches are used. The presented decoupling technique separates equations for each continuum that can be solved separately, leading to a more efficient computational algorithm with smaller systems and faster solutions. This approach is based on the additive representation of the operator with semi-implicit approximation by time, where the continuum coupling part is taken from the previous time layer. We extend and investigate this approach for multiscale approximation on the coarse grid using the nonlocal multicontinuum method. We show that the decoupled schemes are stable, accurate, and computationally efficient.

# [02440] Advances in Optimization I

**Session Time & Room :**

02440 (1/3) : 2D (Aug.22, 15:30-17:10) @A502

02440 (2/3) : 2E (Aug.22, 17:40-19:20) @A502

02440 (3/3) : 3C (Aug.23, 13:20-15:00) @A502

**Type :** Proposal of Minisymposium

**Abstract :** The two minisymposia on Advances in Optimization I and II will bring together a diverse group of leading researchers and practitioners from both continuous and combinatorial optimization, theoretical and applied. One of the goals of these two minisymposia is to raise awareness to the most recent advances in optimization theory, algorithms, and applications, and to develop connections and encourage collaboration.

**Organizer(s) :** Antoine Deza, Takashi Tsuchiya

**Classification :** 90Cxx, 49Mxx, 65Kxx, 52Bxx, 52Cxx

**Minisymposium Program :**

02440 (1/3) : 2D @A502 [Chair: Takashi Tsuchiya]

## [04074] Some Recent Developments on Solving Variational Inequality Problems

**Format :** Talk at Waseda University

**Author(s) :** Shuzhong Zhang (University of Minnesota)

**Abstract :** In this talk, we will present several solution methods for solving non-monotone VI problems. As the VI formulation is generalized from the optimality condition for optimization, the results are immediately applicable to nonconvex and constrained continuous optimization. The focus is placed on the conditions of the non-monotone VI models, under which the newly designed solution algorithms would converge with guaranteed rates of convergence.

## [05227] Monotone Variational Inequality (VI) for estimation and learning

**Format :** Talk at Waseda University

**Author(s) :** Yao Xie (Georgia Institute of Technology)

**Abstract :** We propose a new computational framework for estimating parameters in generalized linear models (GGLMs), inspired by Juditsky and Nemirovsky's recent work. First, we extend GLMs to spatio-temporal data by accounting for dependencies among observations while using a monotone operator-based variational inequality method. We also present online instance-based bounds using martingale concentration inequalities and apply our algorithm to wildfire and police datasets. In addition, we demonstrate our approach to training neural networks.

## [04577] Implementation of Interior Point Method for Nonlinear Programming for Real-life Applications.

**Format :** Talk at Waseda University

**Author(s) :** Takahito Tanabe (NTT DATA Mathematical Systems Inc.)

**Abstract :** In the modeling of real-life applications, we encounter some non-linearity.

In such a case, interior-point algorithm is one approach to choose because it is good at finding locally optimal solutions quickly for large-scale mildly nonlinear problems.

In this talk, we discuss some implementation issues related to interior-point method that originates from non-linearity, and review some applications.

## [04650] Tropical convexity: application to linear programming and mean-payoff games

**Format :** Talk at Waseda University

**Author(s) :** Stephane Louis Gaubert (INRIA and Ecole polytechnique)

**Abstract :** Tropical geometry sets up a bridge between linear programming and mean-payoff games, exploiting a correspondence between generic convex semi-algebraic programs over nonarchimedean fields and different classes of zero-sum repeated games. We will discuss the application of this correspondence to the complexity analysis of interior point methods, showing in particular that no self-concordant barrier interior point method is strongly polynomial. This is based on a series of works with Allamigeon, Benchimol, Joswig and Vandame.

02440 (2/3) : 2E @A502 [Chair: Marcia Fampa]

## [04479] Breaking the quadratic gap for strongly polynomial solvers to combinatorial linear programs

**Format :** Talk at Waseda University

**Author(s) :** Bento Natura (Georgia Tech)

**Abstract :** Recent years have seen tremendous progress in high-accuracy solvers for Maximum Flow, Minimum-Cost Flow and general Linear Programs (LP). Progress on strongly polynomial solvers for combinatorial LP on the other hand has stalled. For combinatorial LP beyond directed graphs this gap between exact and high-accuracy solvers is currently quadratic. We finally break the quadratic gap and design a strongly polynomial interior-point-method for combinatorial LP, which reduces the gap to only a linear factor.

## [03172] Computational challenges in Flag Algebra proofs

**Format :** Talk at Waseda University

**Author(s) :** Aldo Kiem (Zuse Institute Berlin) Sebastian Pokutta (ZIB / TUB) Christoph Spiegel (Zuse Institute Berlin)

**Abstract :** Introduced by Razborov in 2007, flag algebras are a potent tool for computer-assisted proofs in extremal combinatorics. They combine first-order logic, model theory, and semidefinite programming to tackle classical Turán and Ramsey theory problems. This talk explores computational challenges, symmetry exploitation, and optimization ideas to broaden the method's scope. We'll demonstrate its practical application by determining the 4-color Ramsey multiplicity of triangles.

## [03673] Improving Lower Bounds for Large Scale QAPs

**Format :** Talk at Waseda University

**Author(s) :** Koichi Fujii (tokyo institute of technology)

**Abstract :** We report our progress on the project for solving large scale quadratic assignment problems (QAPs).

Our main approach to solve QAPs is a parallel branch-and-bound method using the Ubiquity Generator framework (UG), utilizing Newton-bracketing method to solve doubly nonnegative cone (DNN) relaxations.

In this talk, we present some preliminary numerical results of DNN-based branch-and-bound method and report the result that we have succeeded to update the lower bounds of instances in QAPLIB.

## [03941] Closing Nonzero Duality Gaps in SDPs through Perturbations

**Format :** Talk at Waseda University

**Author(s) :** Takashi Tsuchiya (National Graduate Institute for Policy Studies)Bruno Lourenço (Institute of Statistical Mathematics)Masakazu Muramatsu (The University of Electro-Communication)Takayuki Okuno (Seikei University)

**Abstract :** Consider a primal-dual pair of SDP with nonzero duality gap. There are arbitrary small perturbations to make the pair strongly feasible with a common primal-dual optimal value  $v$ , say, zeroing duality gap.  $v$  is not well-defined at zero (unperturbed problem) since the primal and dual have different optimal values, but it is continuous elsewhere. We analyze properties of  $v$  around zero to demonstrate a few surprising and beautiful properties and establish connections to interior-point methods.

02440 (3/3) : 3C @A502 [Chair: Hiroshi Hirai]

## [04092] Maximum-Entropy Sampling: Algorithms and Application

**Format :** Talk at Waseda University

**Author(s) :** Jon Lee (University of Michigan)Marcia Fampa (Federal University of Rio de Janeiro)

**Abstract :** The maximum-entropy sampling problem (MESP) is to select a subset, of given size  $s$ , from a set of correlated Gaussian random variables, so as to maximize the differential entropy. MESP sits at the intersection of optimization, data science and information theory, and so it has attracted a lot of recent attention. We will give a broad overview of algorithmic work, concentrating on the many useful techniques related to various convex relaxations.

## [03117] A role of semidefinite relaxation in mathematics of phase retrieval

**Format :** Talk at Waseda University

**Author(s) :** Ryoko Oishi-Tomiya (Kyushu University)

**Abstract :** In phase retrieval, a signal  $x$  is recovered from the amplitude  $|Ax|$  for a fixed linear operation  $A$  such as the Fourier transform. In crystallography,  $x$  is a sum of finitely many Gaussian-like functions that represents the periodic discrete structure of atoms. We introduce that semidefinite relaxation works to determine the uniqueness of solutions and gain all the global solutions in this type of problem, mentioning an application found in a joint work with scientists.

## [03176] Exact Convergence Rate of Alternating Projections

**Format :** Talk at Waseda University

**Author(s) :** Yoshiyuki Sekiguchi (Tokyo University of Marine Science and Technology)Hiroyuki Ochiai (Kyushu University)Hayato Waki (Kyushu University)

**Abstract :** We investigate the exact convergence rate of alternating projections for the nontransversal intersection of  $S_+^n$  and an affine space. When the affine space is a line, we analyze the Newton polygon associated with the characteristic polynomial of the parametrizing matrix of the line and show that the convergence rate can be estimated by comparing ranks of submatrices of the basis matrix. We also investigate alternating projections for  $S_+^3$  and a three dimensional affine space.

## [05522] Bridging Distributional and Risk-sensitive Reinforcement Learning with Provable Regret Bounds

**Format :** Talk at Waseda University

**Author(s) :** Zhiqian Luo Zhi-Quan Luo (The Chinese University of Hong Kong, Shenzhen)

**Abstract :** Risk-sensitive decision-making is vital in high-stakes fields like finance and medicine. Risk-sensitive reinforcement learning maximizes a risk measure instead of expected return. The exponential risk measure is widely used but involves complex algorithms and regret analysis. We propose a novel distributional reinforcement learning (DRL) algorithm for RSRL with a regret guarantee. Our approach utilizes risk-sensitive distributional dynamic programming and provides a regret upper bound via distributional optimism, while fixing and tightening the minimax lower bound.

## [02445] Advances in Optimization II

**Session Time & Room :**

02445 (1/3) : 3D (Aug.23, 15:30-17:10) @A502

02445 (2/3) : 3E (Aug.23, 17:40-19:20) @A502

02445 (3/3) : 4C (Aug.24, 13:20-15:00) @A502

**Type :** Proposal of Minisymposium

**Abstract :** The two minisymposia on Advances in Optimization I and II will bring together a diverse group of leading researchers and practitioners from both continuous and combinatorial optimization, theoretical and applied. One of the goals of these two minisymposia is to raise awareness to the most recent advances in optimization theory, algorithms, and applications, and to develop connections and encourage collaboration.

**Organizer(s) :** Antoine Deza, Takashi Tsuchiya

**Classification :** 90Cxx, 49Mxx, 65Kxx, 52Bxx, 52Cxx

**Minisymposium Program :**

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02445 (1/3) : 3D @A502 [Chair: Zhi-Quan Luo]

## [05543] Optimal Diagonal Preconditioning: Theory and Practice

**Format :** Talk at Waseda University

**Author(s) :** Yinyu Ye (Stanford University)

**Abstract :** Preconditioning has long been a staple technique in optimization, often applied to reduce the condition number of a matrix and to speed up the convergence of algorithms. Although there are many popular preconditioning techniques in practice, most lack guarantees on reductions in condition number, and the degree to which we can improve over existing heuristic preconditioners remains an important question. In this paper, we study the problem of optimal diagonal preconditioning, that achieves maximal reduction in the condition number of any full-rank matrix by scaling its rows and/or columns with positive numbers. We first reformulate the problem as a quasi-convex optimization problem and provide a simple algorithm based on bisection. Then we develop an interior point algorithm with  $O(\log(1/\epsilon))$  iteration complexity. Next, we specialize to one-sided optimal diagonal preconditioning problems, and demonstrate that they can be formulated as standard dual SDP problems. We then develop efficient customized solvers for the SDP approach and study the empirical performance of our optimal diagonal preconditioning procedures through extensive experiments. Our findings suggest that optimal diagonal preconditioners can significantly improve upon existing heuristics-based diagonal preconditioners at reducing condition numbers, and our SDP approach can find such optimal preconditioners efficiently for large matrices. We also extend our SDP approach to compute optimal mixtures of base preconditioners, which further improves its scalability and applicability.

## [03259] Smart Initial Basis Selection for Linear Programs

**Format :** Talk at Waseda University

**Author(s) :** Yong Zhang (Huawei Technologies Canada Co., Ltd)

**Abstract :** The simplex method, introduced by Dantzig more than half a century ago, is still to date one of the most efficient methods for solving large-scale linear programming (LP) problems. While the simplex method is known to have the finite termination property under mild assumptions, the number of iterations until optimality largely

depends on the choice of initial basis. Existing strategies for selecting an advanced initial basis are mostly rule-based. These rules usually require extensive expert knowledge and empirical study to develop. Yet, many of them fail to exhibit consistent improvement, even for LP problems that arise in a single application scenario. In this paper, we propose a learning-based approach for initial basis selection. We employ graph neural networks as a building block and develop a model that attempts to capture the relationship between LP problems and their optimal bases. In addition, during the inference phase, we supplement the learning-based prediction with linear algebra tricks to ensure the validity of the generated initial basis. We demonstrate through extensive experiments with state-of-the-art simplex solvers that the proposed strategy can achieve substantial speedup and consistently outperforms existing rule-based methods. Furthermore, we extend the proposed approach to generating restricted master problems for column generation methods and present encouraging numerical results.

## [04683] Interior Point Methods are Not Worse Than Simplex

**Format :** Talk at Waseda University

**Author(s) :** Daniel Dadush (CWI)Xavier Allamigeon (Inria, CMAP, CNRS, Ecole Polytechnique)Bento Natura (Georgia Tech)Georg Loho (University of Twente)Laszlo Vegh (London School of Economics)

**Abstract :** We develop a path-following IPM whose number of iterations is at most  $O(n^{1.5} \log n)$  times the number of segments of any piecewise linear curve traversing the wide neighborhood of the central path. Our IPM matches the number of iterations of any path following IPM up to this polynomial factor and admits an  $O(2^n n^{1.5} \log n)$  upper bound. The latter result complements an exponential lower bound of Allamigeon et al (SIAGA 18) for IPMs.

## [03175] Analysis of Algorithms on Growing Networks

**Format :** Talk at Waseda University

**Author(s) :** Shuji Kijima (Shiga University)

**Abstract :** Real networks are often dynamic. Nevertheless, very few is known about the theoretical analysis of algorithms on dynamic networks. This talk is concerned with some analysis techniques for dynamics on networks with a moderately increasing number of vertices regarding the growing speed.

02445 (2/3) : 3E @A502 [Chair: Stéphane Gaubert]

## [03367] Two constructive techniques for producing linear extended formulations

**Format :** Talk at Waseda University

**Author(s) :** Yuri Faenza (Columbia University)

**Abstract :** We will present two constructive techniques for producing extended formulations: one based on communication protocols, the other on Birkhoff's representation theorem for finite distributive lattices. We also show applications to some problems, mostly in combinatorial optimization.

## [03641] Interior-point methods on manifolds: theory and applications

**Format :** Talk at Waseda University

**Author(s) :** Hiroshi Hirai (Nagoya University)Harold Nieuwboer (University of Amsterdam)Michael Walter (Ruhr University)

**Abstract :** We extend the theory of self-concordance for manifolds, and establish analogous results as in the Euclidean setting, such as quadratic convergence of Newton's method and polynomial iteration complexity of the path-following method. We show that on symmetric spaces of nonpositive curvature, the squared distance function to a point is self-concordant. These results are applied to norm minimization problems for reductive group actions, and to other geometric problems, such as minimum enclosing balls and geometric medians.

## [03069] Alternating Linear Minimization: Revisiting von Neumann's alternating projections

**Format :** Talk at Waseda University

**Author(s) :** Gábor Braun (ZIB)Sebastian Pokutta (ZIB / TUB)Robert Weismantel (ETH)

**Abstract :** In 1933 von Neumann proved a beautiful result that one can compute a point in the intersection of two convex sets (under suitable assumptions) by alternating projections, i.e., successively projecting on one set and then the other. This algorithm assumes that one has access to projection operators for both sets. Here we consider the much weaker setup where we have only access to linear minimization oracles over the convex sets and present

an algorithm to find a point in the intersection of two convex sets. Moreover, we provide a modification of the algorithm to minimize a linear function over the intersection and discuss further extensions.

## [03052] Combinatorial and geometric aspects of linear optimization

**Format :** Talk at Waseda University

**Author(s) :** Antoine Deza (McMaster University)

**Abstract :** Worst-case constructions have helped providing a deeper understanding of how the structural properties of the input affect the computational performance of linear optimization. Recent examples include the construction of Allamigeon et al. for which the interior point method performs an exponential number of iterations. In a similar spirit, recent lower bounds on the number of simplex pivots required in the worst-case to perform linear optimization over a lattice polytope are presented.

02445 (3/3) : 4C @A502 [Chair: Hiroshi Hirai]

## [05126] On Some Optimization-Related Issues In Deep Learning

**Format :** Talk at Waseda University

**Author(s) :** Yin Zhang (The Chinese University of Hong Kong (Shenzhen))

**Abstract :** Despite many great advances achieved by deep learning, our understandings of it remain sorely limited. In this talk, we discuss a few optimization-related issues in deep learning, including model trainability, gradient stability, over-parameterization, quality of (globally optimal) solutions, interpolation versus extrapolation. We will introduce a new neural-layer architecture using Householder weighting and Absolute-value activating that has a low complexity but guarantees gradient stability and 1-Lipschitz continuity. We empirically evaluate the capacities of the proposed new layer and demonstrate its potential usefulness.

## [03071] Creating Collaborative Data Representations Using Matrix Manifold Optimization

**Format :** Talk at Waseda University

**Author(s) :** Keiyu Nosaka (University of Tsukuba)Akiko Yoshise (University of Tsukuba)

**Abstract :** The trade-off between performance and privacy is a pain in the neck for centralized machine learning methods. Fed-DR-Filter and Data Collaboration Analysis (DCA) can overcome this difficulty through Collaborative Data Representation (CDR). We propose an alternative algorithm for CDR creation, utilizing matrix manifold optimization. We devise machine learning models in the DCA setting to evaluate algorithms. The results show that our algorithm outperforms the state-of-the-art approach in mean recognition performance within acceptable computation time.

## [03047] Accelerated and Sparse Algorithms for Approximate Personalized PageRank

**Format :** Talk at Waseda University

**Author(s) :** David Martinez-Rubio (Zuse Institute Berlin)Elias Wirth (Zuse Institute Berlin)Sebastian Pokutta (Zuse Institute Berlin)

**Abstract :** It has recently been shown that ISTA, an unaccelerated optimization first-order method, presents sparse updates for the  $\ell_1$ -regularized personalized PageRank problem, leading to cheap iteration complexity.

In this talk I'll explain our work on accelerated optimization algorithms for this problem that also perform sparse updates leading to faster convergence for certain parameter regimes.

Further, we design a conjugate directions algorithm that achieves an exact solution while exploiting sparsity.

Our findings apply beyond PageRank and work for any quadratic objective whose Hessian is a positive-definite  $M$ -matrix.

## [04893] Optimal Composition Ordering for Linear Functions

**Format :** Talk at Waseda University

**Author(s) :** Kazuhisa Makino (Kyoto Univ.)

**Abstract :** We outline the composition ordering problem of linear functions, i.e., given  $n$  linear functions  $f_1, \dots, f_n : \mathbb{R} \rightarrow \mathbb{R}$  and a constant  $c \in \mathbb{R}$ , we construct a permutation  $\sigma : [n] \rightarrow [n]$  that minimizes  $f_{\sigma(n)} \circ f_{\sigma(n-1)} \circ \dots \circ f_{\sigma(1)}(c)$ , where  $[n] = \{1, \dots, n\}$ .

We discuss structural properties of optimal solutions for the problem as well as the current status of the complexity issue. We also consider the multiplication ordering of  $n$  matrices.

## [02447] Advances in Diesel Engine Design and Control for Industry 4.0

### **Session Time & Room :**

02447 (1/3) : 5B (Aug.25, 10:40-12:20) @E819

02447 (2/3) : 5C (Aug.25, 13:20-15:00) @E819

02447 (3/3) : 5D (Aug.25, 15:30-17:10) @E819

**Type :** Proposal of Minisymposium

**Abstract :** With the advent of Industry 4.0, the demand for efficient and eco-friendly engines has increased. This mini-symposium will present recent research in diesel engine design and control to address the challenges and opportunities of Industry 4.0. Speakers will describe current directions of research and methods relating to optimal nozzle design, combustion limits investigation, intake plenum design improvement, in-cylinder combustion investigation, distinguishability of linear control systems, GAs based PID controller parameter tuning, XAI-based fault diagnosis, and intelligent control systems. The symposium will be of interest to those working in the field of diesel engines and related areas.

**Organizer(s) :** Prof. Dr. Khalid Saifullah, Dr. Athar Kharal

**Classification :** 74A99, 74M05

### **Minisymposium Program :**

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02447 (1/3) : 5B @E819

## [03642] XAI Based Fault Diagnosis for Steel Plates Manufacturing

**Author(s) :** Athar Kharal (Center for Advanced Studies in Pure and Applied Mathematics (CASPAM), Bahauddin Zakariya University, Multan)

**Abstract :** This work uses Explainable Artificial Intelligence tools to develop a fault diagnosis classifier for steel plates. By incorporating insights from techniques such as Ceteris Paribus, Partial Dependence and Breakdown profiles, IF-THEN rules, and an optimized Random Forest and Association Rule Mining, the methodology sought to achieve a high performance using a single ensemble classifier. The methodology is based on medoids and SMOTE and provides valuable insights for experts in the steel manufacturing industry.

## [04142] Distinguishability of linear control systems

**Author(s) :** Awais Younus (CASPAM, BZU, Multan) Zoubia Dastgeer (CASPAM, BZU, Multan)

**Abstract :** Consideration of the observabilities of linear hybrid descriptor systems implies the distinguishability of these systems to be imperative. We have obtained some results related to the distinguishability of the descriptor systems. Also, we have attained equivalent criteria for input distinguishability of descriptor systems with a regular pencil.

## [04661] Optimizing Flow Parameters in Convergent Diesel Nozzles with Rough Walls

**Author(s) :** Khalid Saifullah Syed (Centre for Advanced Studies in Pure and Applied Mathematics, Bahauddin Zakariya University, Multan) Ms Saima Zainab (The Women University, Multan)

**Abstract :** Fuel injector nozzle geometry affect the diesel engine spray and combustion characteristics. This paper explores the effects of nozzle geometry parameters, wall roughness parameters and pressure difference on swirl number, mass flow rate, turbulent kinetic energy and vapor volume fraction. Large-eddy simulations and k- $\omega$  SST Transient models are used to validate the modelling approach. Response Surface Method and Design of Experiment are used to optimize swirl number, turbulent kinetic energy and their linear combination.

## [04696] In-Cylinder Combustion Investigation Against Some Injection Characteristics

**Author(s)** : Anam Ali (CASPAM BZU Pakistan) Khalid Saifullah Syed (Centre for Advanced Studies in Pure and Applied Mathematics, Bahauddin Zakariya University, Multan)

**Abstract** : This study investigates the impact of fuel injection timing and spray angle on combustion characteristics of a heavy-duty diesel engine. CFD simulations are carried out by employing appropriate models to represent different physical and chemical processes. These parameters have significant role in engine design for enhanced combustion efficiency and engine performance. Late injection results into relatively smooth burning rates and considerably lower temperature and pressure peaks without significantly compromising the combustion quality and engine power.

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02447 (2/3) : 5C @E819

## [04704] An Intelligent Control System for a Diesel Engine 1

**Author(s)** : Amna Batool Syeda (Mphil scholar, Center For Advanced Studies in Pure and Applied Mathematics, BZU Multan, Pakistan) Khalid Saifullah Syed (Director of Center for Advanced Studies in Pure and Applied Mathematics, BZU Multan, Pakistan )

**Abstract** : We consider the design of an intelligent, efficient, optimal, robust and hybrid control system based on the adaptive neuro-fuzzy inference system and PID controllers. The system will control air, fuel and EGR for optimal performance and minimum emissions. The system design may involve deep learning of recurrent neural network having several hidden layers with LSTM layer to make the system efficient and more accurate. Optimal control may be incorporated using quadratic programming / genetic algorithm.

## [04750] In-Cylinder Combustion Investigation Against Some Injection Characteristics

**Author(s)** : Khalid Saifullah Syed (Centre for Advanced Studies in Pure and Applied Mathematics, Bahauddin Zakariya University, Multan) Anam Ali (CASPAM BZU Pakistan)

**Abstract** : This study investigates the impact of fuel injection timing and spray angle on combustion characteristics of a heavy-duty diesel engine. CFD simulations are carried out by employing appropriate models to represent different physical and chemical processes. These parameters have significant role in engine design for enhanced combustion efficiency and engine performance. Late injection results into relatively smooth burning rates and considerably lower temperature and pressure peaks without significantly compromising the combustion quality and engine power.

## [04780] In-Cylinder Combustion Investigation Against Some Injection Characteristics

**Author(s)** : Khalid Saifullah Syed (Centre for Advanced Studies in Pure and Applied Mathematics, Bahauddin Zakariya University, Multan) Anam Ali (CASPAM BZU Pakistan)

**Abstract** : This study investigates the impact of fuel injection timing and spray angle on combustion characteristics of a heavy-duty diesel engine. CFD simulations are carried out by employing appropriate models to represent different physical and chemical processes. These parameters have significant role in engine design for enhanced combustion efficiency and engine performance. Late injection results into relatively smooth burning rates and considerably lower temperature and pressure peaks without significantly compromising the combustion quality and engine power.

## [04965] Intake Plenum Design Improvement for a 12-Cylinder Diesel Engine

**Author(s)** : Ms Saima Zainab (The Women University, Multan ) Khalid Saifullah Syed (Centre for Advanced Studies in Pure and Applied Mathematics, Bahauddin Zakariya University, Multan)

**Abstract** : The air flow in engine plenum is complex due to multidimensionality and transient nature of engine operation. This study describes the design modification of intake plenum geometry of a V12 diesel engine and analyses the effects on flow parameters. The original design was found to have strict limits, making it difficult to enhance engine efficiency. However, the modified design is more energy efficient, with greater volumetric efficiency, increased mass flow rate, and turbulent kinetic energy.

02447 (3/3) : 5D @E819

## [05053] Numerical Investigation of HCCI Combustion in the High Pressure Engine

**Author(s)** : Rafia Waqar (Bahauddin Zakariya University, Multan) Khalid Saifullah Syed (Centre for Advanced Studies in Pure and Applied Mathematics, Bahauddin Zakariya University, Multan)

**Abstract** : This study numerically investigates Homogeneous Charge Compression Ignition (HCCI) combustion in a heavy duty engine operating at 4 MPa boosted intake pressure. Effect of variations in charge composition and temperature on combustion performance parameters such as indicated mean effective pressure, indicated torque, indicated power, indicated specific fuel consumption and fuel efficiency are analyzed. Maximum fuel efficiency (~ 47%) is obtained for equivalence ratios between 0.09 – 0.2 for initial temperatures 350 K and 400 K.

## [02448] Verified Numerical Computations and Applications

**Session Time & Room :**

02448 (1/4) : 2C (Aug.22, 13:20-15:00) @E604

02448 (2/4) : 2D (Aug.22, 15:30-17:10) @E604

02448 (3/4) : 2E (Aug.22, 17:40-19:20) @E604

02448 (4/4) : 3C (Aug.23, 13:20-15:00) @E604

**Type** : Proposal of Minisymposium

**Abstract** : In recent decades, the concept of verified numerical computations and computer-assisted proofs is gaining increasing attention and importance.

These methods prove mathematically rigorous results using a combination of analytical arguments such as fixed-point theorems and numerical computations.

This minisymposium focuses on some general tools of accurate and verified numerical computations for the solution of linear and nonlinear systems and eigenvalue problems together with their applications to the proof of solvability and uniqueness for ordinary and partial differential equations.

New developments in that area will be presented.

**Organizer(s)** : Takeshi Ogita, Katsuhisa Ozaki, Siegfried M. Rump, Kazuaki Tanaka

**Classification** : 65G20, 65G40, Verified Numerical Computations

**Minisymposium Program :**

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02448 (1/4) : 2C @E604 [Chair: Siegfried M. Rump]

## [02902] High relative accuracy computing with the Cauchon algorithm

**Format** : Talk at Waseda University

**Author(s)** : Juergen Garloff (University Konstanz) Mohammad Adm (Palestine Polytechnic University Hebron) Fatima Rasheed (Palestine Polytechnic University Hebron)

**Abstract** : We present the condensed form of the so-called Cauchon Algorithm and reformulate the computations in such a way that they can be performed without any subtraction of numbers of equal sign. This provides the basis for an algorithm needing  $O(n^3)$  arithmetic operations for the computation of all eigenvalues of an  $n$ -by- $n$  nonsingular totally nonnegative matrix, i.e., a matrix having all its minors nonnegative, with guaranteed high relative accuracy, independently of the condition number of the matrix.

## [03658] Floating-point matrices with specified solutions for linear algebra problems

**Format** : Talk at Waseda University

**Author(s)** : Katsuhisa Ozaki (Shibaura Institute of Technology) Yuki Uchino (Shibaura Institute of Technology) Takeshi Terao (Kyushu University)

**Abstract** : This research aims to rigorously verify the accuracy of the numerical results for numerical linear

part\_2

algebra problems. If an exact solution to a problem is known in advance, we can observe the relative error of the computed result. We proposed methods that generate a test problem based on an error-free transformation of floating-point numbers. We focus on liner systems, eigenvalue decomposition, singular value decomposition, and least squares problems with specified solutions.

## [05571] Adaptive precision sparse matrix-product and application to Krylov solvers

**Format :** Online Talk on Zoom

**Author(s) :** Stef Graillat (LIP6, Sorbonne Université)Fabienne Jezequel (LIP6, Sorbonne Université)Theo Mary (Sorbonne Université, CNRS, LIP6)Romeo Molina (Sorbonne Université, CNRS)

**Abstract :** We introduce a mixed precision algorithm for computing sparse matrix-vector products and use it to accelerate the solution of sparse linear systems by iterative methods. Our approach is based on the idea of adapting the precision of each matrix element to their magnitude: we split the elements into buckets and use progressively lower precisions for the buckets of progressively smaller elements. We carry out a rounding error analysis of this algorithm that provides us with an explicit rule to decide which element goes into which bucket and allows us to rigorously control the accuracy of the algorithm. We implement the algorithm on a multicore computer and obtain significant speedups (up to a factor 7×) with respect to uniform precision algorithms, without loss of accuracy, on a range of sparse matrices from real-life applications. We showcase the effectiveness of our algorithm by plugging it into various Krylov solvers for sparse linear systems and observe that the convergence of the solution is essentially unaffected by the use of adaptive precision.

## [05577] Iterative refinement for an eigenpair subset of real symmetric matrices

**Format :** Talk at Waseda University

**Author(s) :** Takeshi Terao (Kyushu University)Toshiyuki Imamura (RIKEN Center for Computational Science)Katsuhisa Ozaki (Shibaura Institute of Technology)

**Abstract :** Numerical computation for eigenvalue decomposition plays a crucial role in many scientific fields, and highly accurate eigenpairs are required in certain domains. A novel method was proposed in this study for the iterative refinement of the eigenpair of a real symmetric matrix, which is based on the Ogita-Aishima method and uses compact WY representation. The proposed method can refine the accuracy of a partial eigenpair without using a full eigenvector matrix.

02448 (2/4) : 2D @E604 [Chair: Yoshitaka Watanabe]

## [05276] Lower Bounds for Smallest Singular-Values of Asymptotic Diagonal Dominant Matrices

**Format :** Talk at Waseda University

**Author(s) :** Shin'ichi Oishi (Waseda University)

**Abstract :** This article presents three classes of real square matrices. They are models of coefficient matrices of linearized Galerkin's equations of first order nonlinear delay differential equations with smooth nonlinearity. This paper shows results of computer experiments stating that the minimum singular values of these matrices are unchanged even if orders of matrices are increased. A theorem is presented based on the Schur complement. Through it, tight lower bounds are derived for the minimum singular values of such three matrices. It is proved that these lower bounds are unchanged even if orders of matrices are increased.

## [05029] Error estimation for the FEM solution with a few bad elements

**Format :** Talk at Waseda University

**Author(s) :** Kenta Kobayashi (Hitotsubashi University)

**Abstract :** In conventional error analysis for the finite element method, even one bad element results in poor error estimation. However, numerical results suggest that a few bad elements do not lead to an increase in error. We have provided theoretical proof for this fact, together with the error estimation, that under certain conditions, the presence of a few bad elements does not worsen the error of the finite element method.

## [03173] Verified Numerical Computations for multiple solutions of the Henon equation

**Format :** Talk at Waseda University

**Author(s) :** Taisei Asai (Waseda University)Kazuaki Tanaka (Waseda University)Shin'ichi Oishi (Waseda University)

**Abstract :** In this talk, we describe a numerical verification of the Henon equation in which some asymmetric solutions arise due to the nonlinear term.

The existence of multiple solutions is verified on various domains, and the relationship between the domain and the symmetry of the solution will be discussed.

## [05290] Rigorous solution-enclosures of elliptic boundary value problems between piecewise linear functions

**Format :** Talk at Waseda University

**Author(s) :** Kazuaki Tanaka (Waseda University)

**Abstract :** Sub- and super-solutions are useful for obtaining stable solutions of elliptic boundary value problems. However, their conventional definition requires smoothness, which makes it difficult to construct sub- and super-solutions using piecewise linear functions. To overcome this issue, we propose a definition that uses a variational inequality and constrained test functions. We show that the generalized sub- and super-solutions enclose the desired solutions, and that even a simple difference method can construct sub- and super-solutions that enclose the true solutions.

02448 (3/4) : 2E @E604 [Chair: Kenta Kobayashi]

## [04361] Verified computation for shape derivative of the Laplacian eigenvalues

**Format :** Talk at Waseda University

**Author(s) :** Ryoki Endo (Niigata University)Xuefeng Liu (Niigata University)

**Abstract :** The shape derivative of Laplacian eigenvalues with respect to domain deformations was theoretically investigated by Hadamard in the early 20th century. However, the rigorous computation of these derivatives is not an easy task, since there exists the singularity for repeated eigenvalues. In this study, we propose a verified computation method for the shape derivative of Laplacian eigenvalues using guaranteed computation of both eigenvalues and eigenfunctions.

## [04568] Constructive error estimates for a full-discretized periodic solution of heat equation

**Format :** Talk at Waseda University

**Author(s) :** Takuma Kimura (Saga University)Teruya Minamoto (Saga University)Mitsuhiro T. Nakao (Waseda University)

**Abstract :** In this talk, we consider the constructive a priori error estimates for a full discrete numerical solution of the heat equation with time-periodic condition;

$$\frac{\partial u}{\partial t} - \nu \Delta u = f(x, t) \text{ in } \Omega \times J, \quad u(x, t) = 0 \text{ on } \partial\Omega \times J, \quad u(x, 0) = u(x, T) \text{ on } \Omega.$$

Our numerical scheme is based on the finite element semi-discretization in space direction combined with the Fourier expansion in time.

Several numerical examples will be shown to illustrate the theoretical results.

## [03685] A Numerical verification method for a self-similar solution to the linear elliptic differential equation

**Format :** Talk at Waseda University

**Author(s) :** Kouta Sekine (Chiba Institute of Technology)Taiyou Fuse (Chiba Institute of Technology)

**Abstract :** In this talk, we propose a numerical verification method for self-similar solutions of linear partial differential equations on ( $\mathbb{R}$ ) using the Galerkin approximation with extended Hermite polynomials. In particular, we derive a Gaussian quadrature method for extended Hermite polynomials to errors in numerical quadrature over infinite interval. Also, we also introduce the projection error constant for obtaining the discretisation error of the Hermite-Galerkin approximation.

## [04321] A computer-assisted proof for a nonlinear differential equation involved with self-similar blowup in wave equations

**Format :** Talk at Waseda University

**Author(s) :** Yoshitaka Watanabe (Kyushu University)Kaori Nagatou (Karlsruhe Institute of Technology)Michael Plum (Karlsruhe Institute of Technology)Birgit Schörkhuber (University of Innsbruck)Mitsuhiro T. Nakao (Waseda University)

**Abstract :** An existence proof with its specific shape of a non-trivial solution of a nonlinear ordinary differential equation involved with self-similar blowup in three-dimensional wave equations is presented. The proof is computer-assisted based on a fixed-point and Newton-type formulation, and the result takes into account the effects of rounding errors of floating-point arithmetic in computer.

02448 (4/4) : 3C @E604

## [02458] Progress and Challenges in Extreme Scale Computing and Big Data

**Session Time & Room :**

02458 (1/3) : 2C (Aug.22, 13:20-15:00) @D101

02458 (2/3) : 2D (Aug.22, 15:30-17:10) @D101

02458 (3/3) : 2E (Aug.22, 17:40-19:20) @D101

**Type :** Proposal of Minisymposium

**Abstract :** Extreme scale computing efforts have resulted in numerous advances for multicore and accelerator based scalable systems. In addition, large-scale applications must increasingly deal with data management and analysis as a first-class concern. Therefore, new applications often have to manage distributed and parallel computing, and have to manage workflows of different tasks, such as computing, data analytics, machine learning, visualization, etc. In this MS, we present some of the latest work in scalable algorithms, programming paradigms, and libraries for next generation computing platforms. Furthermore, we discuss efforts to better incorporate data science concerns as an important component of our scientific workflows.

**Organizer(s) :** Keng Nakajima, Michael Heroux, Serge Petiton

**Classification :** 68W10, 65Y05, Computational Science, Numerical Algorithms, Data Analytics, Machine Learning, High-Performance Computing

**Minisymposium Program :**

02458 (1/3) : 2C @D101 [Chair: Kengo Nakajima]

## [05261] Toward Post-Exascale Software-Ecosystem Sustainment

**Format :** Talk at Waseda University

**Author(s) :** Michael Heroux (Sandia National Labs)

**Abstract :** The US Department of Energy (DOE) Exascale Computing Project (ECP) is ending soon. ECP exhibited the value of sustained and coordinated software development and delivery and DOE is exploring approaches to sustain the ecosystem that ECP produced.

In this talk, we discuss some of the key goals and strategies under consideration for post-ECP software-ecosystem sustainment. We consider organizational and collaboration strategies, processes, and tools that can help the community realize sustainment beyond the end of ECP.

## [03388] Task-based hybrid parallel matrix factorization for distributed memory environment

**Format :** Talk at Waseda University

**Author(s) :** Tomohiro Suzuki (University of Yamanashi University)

**Abstract :** The task parallel approach provided by OpenMP has achieved great success in shared memory environments. In distributed memory environments, an interoperability issue exists between MPI and OpenMP. Several techniques have been proposed to address the issue. However, these proposed methods require a high level of thread support in MPI, so they can only work in limited environments.

In this presentation, basic experimental results performed on the Wisteria-O system will be presented.

## [03651] Accelerating lattice Boltzmann method with GPU and C++ standard parallelization

**Format :** Talk at Waseda University

**Author(s) :** Ziheng Yuan (The University of Tokyo)Takashi Shimokawabe (The University of Tokyo)

**Abstract :** In recent years, with the increasing use of GPUs as accelerators in the HPC platform, using C++ standard parallel language as a GPU programming language has also attracted attention. Compared with traditional parallel programming languages, C++ standard parallel language for programming has advantages such as readability and maintainability of the code. This talk intends to introduce the application of C++ standard parallel language in fluid simulation using the lattice kinetic scheme (LKS), an extended lattice Boltzmann method (LBM), and discusses its performance.

## [05041] GPU-accelerated viscoelastic crustal deformation analysis with data-driven method

**Format :** Talk at Waseda University

**Author(s) :** Sota Murakami (The University of Tokyo)Kohei Fujita (The University of Tokyo)Tsuyoshi Ichimura (The University of Tokyo)Takane Hori (Japan Agency for Marine-Earth Science and Technology)Muneo Hori (Japan Agency for Marine-Earth Science and Technology)Maddegedara Lalith (The University of Tokyo)Naonori Ueda (RIKEN)

**Abstract :** We developed a viscoelastic analysis solver with data-driven method on GPUs for fast computation of highly detailed 3D crustal structure models. Here, the initial solution is obtained with high accuracy using a data-driven predictor based on previous time-step results, which reduces the number of multi-grid solver iterations and thus reduces the computation cost. The algorithm is designed to be suitable for GPUs. The developed GPU-based solver attained 8.6-fold speedup from the state-of-art GPU-based multi-grid solver.

02458 (2/3) : 2D @D101 [Chair: Kengo Nakajima]

## [03035] System-Wide Coupling Communication for Heterogeneous Computing Systems

**Format :** Talk at Waseda University

**Author(s) :** Shinji Sumimoto (The University of Tokyo)Takashi Arakawa (CliMTech Inc.)Yoshio Sakaguchi (Fujitsu Ltd.)Hiroya Matsuba (Hitachi Ltd.)Satoshi Ohshima (Kyushu University)Hisashi Yashiro (National Institute for Environmental Studies)Toshihiro Hanawa (The University of Tokyo)Kengo Nakajima (The University of Tokyo/RIKEN)

**Abstract :** This talk presents a system-wide coupling communication library to couple multiple MPI programs for heterogeneous coupling computing called h3-Open-SYS/WaitIO (WaitIO for short). WaitIO provides an inter-program communication environment among MPI programs and supports different MPI libraries with various interconnects and processor types. We have developed the WaitIO communication library to realize the environments. We present how WaitIO works and performs in such heterogeneous computing environments.

## [03261] h3-Open-UTIL/MP: a coupling library for heterogeneous computing

**Format :** Talk at Waseda University

**Author(s) :** Takashi Arakawa (The University of Tokyo)Shinji Sumimoto (The University of Tokyo)Hisashi Yashiro (National Institute for Environmental Studies)Kengo Nakajima (The University of Tokyo/RIKEN)

**Abstract :** Heterogeneous computing is one of the main topics for recent high-performance computing. The reason is that role of HPC has expanded beyond not only simple simulation but also to large-scale data analysis and machine learning. Based on these backgrounds, we are developing a heterogeneous coupling library h3-Open-UTIL/MP. In our presentation, we will describe the structure and function of h3-Open-UTIL/MP and discuss the results of performance measurements and application examples.

## [03652] Modernizing the weather prediction model ICON for extreme-scale computing, a librarization effort

**Format :** Talk at Waseda University

**Author(s) :** Yen-Chen Chen (Karlsruhe Institute of Technology)Terry Cojean (Karlsruhe Institute of Technology)Jonas Jucker (CSCS Swiss National Supercomputing Centre)Pradipta Samanta (German Climate Computing Centre)Florian Prill (Deutscher Wetterdienst)Sergey Kosukhin (Max-Planck-Institute for Meteorology)Luis Kornblueh (Max-Planck-Institute for Meteorology)Will Sawyer (CSCS Swiss National Supercomputing Centre)Jörg Behrens (German Climate Computing Centre)Claudia Frauen (German Climate Computing Centre)

**Abstract :** The weather and climate prediction model ICON was operated since 1999 and has become the forecasting model of more than 30 national weather services. However, the legacy Fortran code restricts its portability to GPU clusters and hinders its parallel performance on modern exascale clusters. The ICON consolidated (ICON-C) project and several related projects aim to make ICON more modular, portable, and suitable for modern extreme-scale parallel computing. This talk focuses on a librarization effort of ICON-C.

## [03776] Performance Modeling Challenges in Extreme Scale Computing

**Format :** Online Talk on Zoom

**Author(s) :** Ayesha Afzal (Erlangen National High Performance Computing Center (NHR@FAU))

**Abstract :** In extreme scale computing, analytic performance modeling using first-principles is pre-eminent for optimization. However, it is challenging since the implicit presumption of strict synchronization among all processes is not necessarily accurate. Therefore, for programs with rare synchronization points, simply summing the runtimes predicted by computation and communication performance models is often erroneous.

In my talk, I will highlight the most intriguing insights about intricate hardware-software interactions emerging from this model failure. Interestingly, the hardware bottlenecks permits for non-intuitive spontaneous asynchronicity that helps to get the most of the systems' capabilities and mitigates the communication overhead.

02458 (3/3) : 2E @D101 [Chair: Kengo Nakajima]

## [05260] Exascale challenges and opportunities for fundamental research

**Format :** Online Talk on Zoom

**Author(s) :** Christophe Calvin (CEA)France Boillod-Cerneux (CEA)Valérie Brenner (CEA)

**Abstract :** With the exascale come new challenges: the processing of massive data coupled with digital simulation becomes intrinsic to science. In addition, the constraints brought by the architectures of calculation for the exascale impose to also rethink the scientific applications. We are therefore faced with two major challenges. The 1st one: how the new exascale calculators, inscribed in a digital continuum, will be able to provide solutions for the processing of complex workflows combining data processing and simulation. The 2nd, how to design or redesign the applications in order to be able to exploit the architectures of the exascale supercomputers. We will illustrate these 2 challenges through different use cases at the CEA's Fundamental Research Division.

## [03605] An algorithm reducing by 2 the number of operations for the PageRank method, and its generalisation for stochastic matrix-vector products

**Format :** Online Talk on Zoom

**Author(s) :** serge georges petiton (University of Lille, CNRS)Maxence Vandromme (RATP Smart Systems)

**Abstract :** We propose an efficient PageRank algorithm that reduces the complexity by a factor two. We implement the method using row-major and column-major sparse matrix formats. The experiments are done on two different Intel processors from recent generations. The column-major storage format version of our method shows good scaling and outperforms the standard PageRank in a majority of cases. We also propose generalisations of this algorithm to the multiplication of stochastic matrices by a vector product.

## [03705] Accelerating Cardiac Electrophysiology Simulations using novel AI Hardware

**Format :** Talk at Waseda University

**Author(s) :** Johannes Langguth (Simula Research Laboratory)Luk Bjarne Burchard (Simula Research Laboratory)Xing Cai (Simula Research Laboratory)

**Abstract :** Recent advances in personalized arrhythmia risk prediction show that computational models can provide not only safer but also more accurate results than invasive procedures. However, biophysically accurate simulations require solving linear systems over fine meshes and time resolutions, which require significant computational resources. However, by leveraging sophisticated parallelization patterns as well as non-traditional hardware architectures, it is possible to meet the computational demands of these simulations.

A major recent development in computer hardware was the rise of dedicated accelerator hardware for machine learning applications such as the Graphcore IPUs and Cerebras WSE. These processors have evolved from the experimental state into market-ready products, and they have the potential to constitute the next major architectural shift after GPUs saw widespread adoption a decade ago.

In this talk, we present ongoing work on the parallelization of finite volume computations over an unstructured mesh using these new accelerators. We compare them to traditional CPUs and GPUs and point out challenges and opportunities of this new hardware for extreme scale computing.

## [05304] A Medical Data Analytics Framework Transforming Big Data to Better Healthcare

**Format :** Talk at Waseda University

**Author(s) :** Weichung Wang (National Taiwan University)

**Abstract :** Incorporating data science is crucial for the next-generation medical workflows that rely on high-performance computing to analyze large-scale medical data for digital and precision medicine. The "Medical Data Analytics Framework" combines project design, multimodality data, intelligent analytics, medical workflows, regulation, ethics, deployment, and operations to achieve an end-to-end R&D life-cycle in medical AI that positively impacts clinical workflows. This interdisciplinary framework reduces physicians' workload and assists in diagnosing with advanced algorithms and software.

## [02470] Chaotic Supremacy Revolution

**Session Time & Room :**

02470 (1/2) : 4C (Aug.24, 13:20-15:00) @G402

02470 (2/2) : 4D (Aug.24, 15:30-17:10) @G402

**Type :** Proposal of Minisymposium

**Abstract :** Chaotic supremacy will be discussed from the perspective of applied mathematics such as applied chaos theory and new device technologies such as laser chaos for terahertz generation and off-shell science. Innovative applied chaos research cases from academia as well as industry, which has been studying applied chaos for many years, will also be presented.

**Organizer(s) :** Ken Umeno, Fumiyoji Kuwashima, (4) Takashi Isoshima

**Classification :** 34H10, 65P20, 34Hxx, Chaos**Minisymposium Program :**

02470 (1/2) : 4C @G402

## [03810] Chaos-like behavior of two-dimensional optical bistable device with external feedback

**Author(s)** : Takashi Isoshima (RIKEN-CPR)

**Abstract** : Bistable system with a spatial expanse can provide a wavefront, an interface between two stable states, that can propagate. We investigate a two-dimensional optical bistable device (2DOBD) based on thermo-optical positive feedback for natural computing including maze exploration. Addition of external feedback to the device can realize complex spatio-temporal behavior. Refractory feedback, inspired by the refractory period of a nerve cell, provides propagating pulse generation, and under some condition, chaotic behavior of the pulses.

## [03967] Quantification of Orbital Instability of Chaotic Laser Diodes by Modified Orbital Expansion Exponent

**Author(s)** : Satoshi Ebisawa (Niigata Institute of Technology)

**Abstract** : Controlling the strength of orbital instability of chaotic laser, is useful for applications. To realize this, it is important to quantify the characteristics. The chaotic laser has three dynamic variables, but only the amplitude can be easily measured experimentally. Then, we introduce a modified orbital expansion exponent that considers the chaotic laser dynamics. By comparing this with the Lyapunov exponent calculated from the rate equations representing its dynamics, we show the usefulness of proposed exponent.

## [03992] Development of MLD-TDS applying spintronic THz emitters excited by laser chaos light

**Author(s)** : Takeshi Moriyasu (University of Fukui)Ryunosuke Noda (University of Fukui)Kaede Miyaguchi (University of Fukui)Shudai Katono (University of Fukui)Masahiko Tani (University of Fukui)Hideaki Kitahara (University of Fukui)Fumiyoji Kuwashima (Fukui University of Technology)Mitsutaka Kumakura (University of Fukui)

**Abstract** : A terahertz time-domain spectrometer with a multimode laser diode as light source (MLD-TDS) is an inexpensive terahertz spectrometer, since an expensive pulse laser system is not used. However, MLD-TDS has not been widely adopted in practical applications due to the sub-optimal radiation efficiency and stability etc. We propose the applying of spintronic THz emitters and laser chaos light into the MLD-TDS system, with the aim of compensating for the deficiencies and enhancing the overall performance.

## [04023] Application of entropic chaos degree to Lorenz system

**Author(s)** : Kei Inoue (Sanyo-Onoda City University)

**Abstract** : The entropic chaos degree was introduced to measure the chaos of a dynamical system in Information Dynamics. It is computable for any time series, even if the dynamical system is unknown. Recently the extended entropic chaos degree was proposed, equal to the total sum of the Lyapunov exponents under typical chaotic conditions. In this study, I try to measure the chaos of the Lorenz system by the extended entropic chaos degree.

02470 (2/2) : 4D @G402

## [04036] Stable THz waves using laser chaos

**Author(s)** : Fumiyoji Kuwashima (Fukui Univ. of Tech.)Mona Jarrahi (Electrical and Computer Engineering Department, University of California Los Angeles)Semih Cakmakyapan (Electrical and Computer Engineering Department, University of California Los Angeles)Osamu Morikawa (Chair of Liberal Arts, Japan Coast Guard Academy)Takuya Shirao (Fukui Univ. of Tech.)Kazuyuki Iwao (Fukui Univ. of Tech.)Kazuyoshi Kurihara (School of Education., University. of Fukui)Hideaki Kitahara (Research Center for Development of Far-Infrared Region, University of Fukui)Takashi Furuya (Research Center for Development of Far-Infrared Region, University of Fukui)Yuki Kawakami ( National Institute of Technology (KOSEN), Fukui College)Takeshi Moriyasu (UniversFaculty of Engineering, University of Fukui)Kenji Wada (Osaka Metropolitan University)Makoto Nakajima (Institute of Laser engineering, Osaka Univ.)Masahiko Tani ( Research Center for Development of Far-Infrared Region)

part\_2

**Abstract :** Efficiency of optical beats in a chaotically oscillating laser is confirmed comparing that of free running CW laser using a highly efficient plasmonic photomixer. The great potential of chaotically oscillating lasers is verified for THz systems. This is one of the proof of Chaotic Supremacy in real system.

### [04083] Quantum walk analysis of spatial distribution of dressed-photon-phonon

**Author(s) :** Motoichi Ohtsu (Research Origin for Dressed Photon)Etsuo Segawa (Yokohama National University)Kenta Yuki (Middenii)Seiken Saito (Kogakuin University)

**Abstract :** This paper analyzes the spatial distribution of a dressed-photon-phonon (DPP) that is confined by a boron (B) atom-pair in a silicon light-emitting diode by using a two-dimensional quantum walk model. It is confirmed that the DPP is confined by the B atom-pair, which is oriented along a direction perpendicular to that of the incident light propagation. The dependence of the confined DPP probability on the length of the B atom-pair is analyzed.

### [04616] Quantum Fields as Category Algebras

**Author(s) :** Hayato Saigo (Nagahama Institute of Bio-Science and Technology)

**Abstract :** In the present talk we propose a new approach to quantum fields in terms of category algebras and states on categories. We define quantum fields and their states as category algebras and states on causal categories with partial involution structures. Based on this framework, we propose a foundation for off-shell sciences such as dressed phonon studies.

### [05241] Exactly Solvable Chaos and Its Use to Realize Chaotic Supremacy

**Author(s) :** Ken Umeno (Kyoto University)

**Abstract :** Theory of exactly solvable chaos, whose ergodic invariant measure is explicitly obtained, is firstly reviewed as a key concept to analyze chaotic supremacy analytically. Superefficient chaotic Monte Carlo computation is one of the key examples to realize chaotic supremacy. Then we discuss a possible relation between chaotic supremacy and quantum supremacy from the view point of the connection of chaotic superefficiency realized by primitive root codes (discretization of exactly solvable chaos) with quantum Grover's algorithm.

## [02474] Applied and Computational Dynamics

**Session Time & Room :**

02474 (1/2) : 2D (Aug.22, 15:30-17:10) @F308

02474 (2/2) : 2E (Aug.22, 17:40-19:20) @F308

**Type :** Proposal of Minisymposium

**Abstract :** Understanding the long-term behaviour of a dynamical system is an important challenge that requires many mathematical techniques and numerical tools. Dynamical systems are models with a natural time evolution (discrete or continuous). The invariant sets (fixed points, periodic orbits, invariant manifolds, strange attractors, etc.) are all objects that persist beyond the transient phase, and thus carry important information. It is also necessary to understand the bifurcations that occur as model parameters are varied. In this minisymposium, we will learn of new results for analyzing dynamical systems. Examples include passive dynamic walking, Fitzhugh-Nagumo neurons, and self-propelled particle systems.

**Organizer(s) :** Warwick Tucker (University of Melbourne, Australia), Yoshitaka Saiki (Hitotsubashi University, Japan), Hiroe Oka (Ryukoku University, Japan), Hiroshi Kokubu (Kyoto University, Japan)

**Classification :** 37Cxx, 37Dxx, 37Nxx, 37Gxx, 28Dxx

**Minisymposium Program :**

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02474 (1/2) : 2D @F308 [Chair: Hiroshi Kokubu]

## [03364] Connectedness of graphs of dynamical systems

**Format :** Talk at Waseda University

**Author(s) :** James A Yorke (Univ. Of Maryland )Roberto De Leo (Howard Univ.)

**Abstract :** We have been developing the general theory of graphs of maps or differential equations that works for maps, ordinary differential equations and parabolic partial differential equations. We have a complete theory for the logistic map.

We have created axioms for graphs that can be used to prove results about graphs, axioms that hold for all of the standard definitions. We prove that the graph is connected under mild hypotheses.

## [03770] Changes in basin of attraction by homoclinic and heteroclinic tangencies in passive dynamic walking

**Format :** Talk at Waseda University

**Author(s) :** Kota Okamoto (Kyoto University)Ippei Obayashi (Okayama University)Hiroshi Kokubu (Kyoto University)Kei Senda (Kyoto University)Kazuo Tsuchiya (Kyoto University)Shinya Aoi (Osaka University)

**Abstract :** In the passive dynamic walking that walks down a shallow slope without any control or input, countless sudden changes appear in the basin of attraction depending on the slope angle. An infinite number of periodic solutions also appear. We investigated the mechanism of the sudden changes in the basin of attraction of the passive dynamic walking based on the homoclinic and heteroclinic tangencies of the manifolds of the periodic solutions.

## [04997] A novel bifurcation in hybrid dynamical systems: a model of human locomotion and its generalization

**Format :** Talk at Waseda University

**Author(s) :** Hidetoshi Morita (Shitennoji University)Shinya Aoi (Osaka University)Kazuo Tsuchiya (Kyoto University)Hiroshi Kokubu (Kyoto University)

**Abstract :** Aiming to understand the coexistence of walk and run in human locomotion, we study a simpler vertical motion of inverted spring-mass model. We observe the coexistence of two limit cycles between which no unstable periodic orbit lies, unlike the usual coexistence of attractors. We analyze the mechanism of this novel type of coexistence. We further consider a generalized hybrid dynamical systems model, and analyze the corresponding, as well as yet other, behaviors.

## [03723] Coupled Hopf bifurcations: interaction between Fitzhugh-Nagumo neurons

**Format :** Talk at Waseda University

**Author(s) :** Fátima Drubi (University of Oviedo)Santiago Ibáñez (University of Oviedo)Diego Noriega (University of Oviedo)

**Abstract :** Coupled dynamical systems allow to model a wide range of phenomena. We are interested in models where identical pieces with simple dynamics are coupled through simple mechanisms, wondering about the complexity that interaction may imply. The coupling of identical families of vector fields exhibiting a Hopf bifurcation is paradigmatic. After discussing a general model, we will focus on the interaction between two Fitzhugh-Nagumo planar systems and study the appearance of Hopf-Pitchfork and Hopf-Hopf bifurcations.

02474 (2/2) : 2E @F308 [Chair: Warwick Tucker]

## [04209] A method of computing Morse decomposition via approximate ODE solvers and its application

**Format :** Talk at Waseda University

**Author(s) :** Tomoyuki Miyaji (Kyoto University)

**Abstract :** Computing Conley--Morse graphs for dynamical systems defined by ordinary differential equations using rigorous ODE solvers such as Lohner's method is suffered from wrapping effects and is computationally expensive. It is especially remarkable when applied to Poincaré maps. In this talk, we apply approximate solvers, such as the Runge--Kutta methods, to computing Morse decomposition. We will discuss its application to Poincaré maps for 4D ODEs arising in modeling the motion of a self-propelled particle.

## [03407] Finite-resolution recurrence in dynamical models

**Format :** Talk at Waseda University

**Author(s) :** Paweł Pilarczyk (Gdansk University of Technology, Faculty of Applied Physics and Mathematics) Justyna Signerska-Rynkowska (Dioscuri Centre in Topological Data Analysis, Institute of Mathematics of the Polish Academy of Sciences) Grzegorz Graff (Gdansk University of Technology, Faculty of Applied Physics and Mathematics)

**Abstract :** In order to improve the method for rigorous analysis of global dynamics based on a set-oriented topological approach, introduced by Arai et al. in 2009 (SIAM J. Appl. Dyn. Syst. 8, 757-789), we introduce the notion of finite-resolution recurrence, develop an effective algorithm for its computation, and apply it to a two-dimensional model of a neuron. We additionally use machine learning to distinguish between different types of dynamics observed.

## [04891] Reconstruction of stationary measures from 'cycles' in random dynamical systems

**Format :** Talk at Waseda University

**Author(s) :** Hiroki Takahasi (Keio Institute of Pure and Applied Sciences)

**Abstract :** One leading idea in the qualitative understanding of deterministic dynamical systems is to use collections of periodic orbits to structure the dynamics. This idea traces back to Poincaré, and has been supported by Bowen who proved that periodic orbits of topologically mixing Axiom A diffeomorphisms equidistribute with respect to the measure of maximal entropy. We consider an analogue of Bowen's equidistribution theorem of periodic orbits in the context of simple random dynamical systems.

## [03823] Computer verifiable criteria for chaos in piecewise smooth dynamical systems

**Format :** Talk at Waseda University

**Author(s) :** Paul Glendinning (University of Manchester)

**Abstract :** Many theoretical results on chaotic behaviour in piecewise smooth maps rely on relatively simple criteria that could in principle be checked by hand. I will describe some of these results and how they can be implemented numerically. This makes it possible to demonstrate the existence of phenomena such as robust chaos and unstable manifold variability in examples. Many of the results presented are from joint work with D.J.W. Simpson (Massey University, New Zealand).

# [02479] Recent advances for modeling, numerical algorithm, and applications in electronic structure calculation

**Session Time & Room :**

02479 (1/3) : 2E (Aug.22, 17:40-19:20) @E711

02479 (2/3) : 3C (Aug.23, 13:20-15:00) @E711

02479 (3/3) : 3D (Aug.23, 15:30-17:10) @E711

**Type :** Proposal of Minisymposium

**Abstract :** With the rapid development of the research in the electronic structure calculations, new mechanisms and phenomenon are constantly being discovered, which bring the challenging on mathematical modeling and related analysis. Meanwhile, the development of the computational hardware also provides chances to the new algorithm design and analysis. In this mini-symposium, experts from mathematics, physics, etc., would share their recent progress in the research of the electronic structure calculations, and will discuss together towards the potential applications in areas such as computational quantum chemistry, nano-optics.

**Organizer(s)** : Zhenning Cai, Guanghui Hu, Hehu Xie

**Classification** : 65N30, 65N25, 65M55, 65Z05

**Minisymposium Program :**

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02479 (1/3) : 2E @E711 [Chair: Guanghui Hu]

## [04686] Numerical method for the Elasticity Transmission Eigenvalues

**Format** : Talk at Waseda University

**Author(s)** : xia ji (Beijing institute of technology )

**Abstract** : We develop a discontinuous Galerkin method computing a few smallest elasticity transmission eigenvalues, which are of practical importance in inverse scattering theory. For high order problems, DG methods are competitive since they use simple basis functions, the numerical implementation is much easier compared with classical conforming finite element methods. In this talk, we propose an interior penalty discontinuous Galerkin method using C0 Lagrange elements (C0IP) for the transmission eigenvalue problem for elastic waves and prove the optimal convergence. The method is applied to several examples and its effectiveness is validated.

## [03287] A multi-mesh adaptive finite element method for Kohn-Sham equation

**Format** : Talk at Waseda University

**Author(s)** : Yang Kuang (Guangdong University of Technology)

**Abstract** : We present a multi-mesh adaptive finite element method for solving the Kohn-Sham (KS) equation. Specifically, the KS equation and the Poisson equation corresponding to the Hartree potential is solved in two different adaptive meshes on the same computational domain. With the presented method, we are able to evaluate the Hartree potential and Hartree energy more accurately, so as to reach a better accuracy with less computational cost in the all-electron calculations.

## [03432] Mathematical theory and numerical methods for Bose-Einstein condensation with higher order interactions

**Format** : Talk at Waseda University

**Author(s)** : Xinran Ruan (Capital Normal University)Weizhu Bao (National University of Singapore)Yongyong Cai (Beijing Normal University)

**Abstract** : The binary interaction in Gross-Pitaevskii equation, which is a big success in describing Bose-Einstein condensate, is typically chosen as Fermi contact interaction. However, in certain cases, higher order interaction (HOI) needs to be included.

In the talk, I will show new phenomenon introduced by HOI, such as the non-Gaussian type approximations in dimension reduction problems , new types of Thomas-Fermi approximations. Besides, two algorithms for computing ground states, which overcome the stability issue, will be presented.

## [03403] Solving Schrodinger equation using tensor neural network

**Format** : Talk at Waseda University

**Author(s)** : Hehu Xie (Academy of Mathematics and Systems Science, Chinese Academy of Sciences)

**Abstract** : In this talk, we introduce a prototype of machine learning method to solve high dimensional partial differential equations by the tensor neural network. Based on the tensor product structure, we can do the direct numerical integration by using fixed quadrature points for the functions constructed by the tensor neural network within tolerable computational complexity. The corresponding machine learning method is built for solving high dimensional Schrodinger equation with high accuracy. Some numerical examples are provided to validate the accuracy and efficiency of the proposed algorithms. This work is collaborated with Yifan Wang and Pengzhan Jin.

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02479 (2/3) : 3C @E711 [Chair: Hehu Xie]

## [04589] Computations of the ground states and collective excitations of Bose-Einstein condensates

**Author(s)** : Manting Xie (Tianjin University)Hehu Xie (Academy of Mathematics and Systems Science, Chinese Academy of Sciences)Yong Zhang (Tianjin University)

**Abstract** : In this talk, we'll show some efficient and robust numerical methods to study the ground states and collective excitations of Bose-Einstein condensates.

## [03384] Multilevel correction adaptive finite element method for Kohn-Sham equation

**Format** : Talk at Waseda University

**Author(s)** : Fei Xu (Beijing University of Technology)

**Abstract** : An efficient adaptive finite element method is proposed for solving the ground state solution of the Kohn-Sham equation which is based on the combination of the multilevel correction scheme and the adaptive refinement technique. The multilevel correction adaptive finite element method can transform the Kohn-Sham equation into a series of linear boundary value problems on the adaptive partitions and a series of Kohn-Sham equations on very low dimensional spaces. Further, the Hartree potential and the exchange-correlation potential are treated individually, and the algorithm can be performed in an eigenpairwise approach. Therefore, the presented adaptive method for Kohn-Sham equation can arrive at the similar efficiency as that of the adaptive finite element method for the associated linear boundary value problems.

## [03227] The Wigner function of ground state and one-dimensional numerics

**Format** : Talk at Waseda University

**Author(s)** : Hongfei Zhan (Peking University)

**Abstract** : In this talk, the ground state Wigner function of a many-body system is explored theoretically and numerically. An eigenvalue problem for Wigner function is derived based on the energy operator of the system. On the other hand, a numerical method is designed for solving proposed eigenvalue problem in one dimensional case. Results of several numerical experiments verify our method, where the potential application for large scale system is demonstrated by examples with density functional theory.

02479 (3/3) : 3D @E711

## [02491] Mathematics of Epidemics: modelling, data analysis, and control

**Session Time & Room** :

02491 (1/2) : 4D (Aug.24, 15:30-17:10) @A201

02491 (2/2) : 4E (Aug.24, 17:40-19:20) @A201

**Type** : Proposal of Minisymposium

**Abstract** : Mathematical epidemiology, the modeling of the spread of epidemics, has a distinguished history and continues to be a very active field, with fruitful interaction of mathematical theory, computation, and data analysis. In the wake of the COVID-19 pandemic, modeling has played an important role in providing a framework for understanding empirical data and guiding policy. This mini-symposium will include presentations of recent results related to the mathematical modeling of epidemics, and provide a forum for discussion among researchers. Issues to be addressed include control measures for epidemics, population immunity and vaccination, heterogeneity of populations, and parameter inference for epidemic models.

**Organizer(s)** : Nir Gavish, Guy Katriel, Yukihiko Nakata

**Classification** : 92D30, 34H05, 92B05

**Minisymposium Program** :

02491 (1/2) : 4D @A201 [Chair: Guy Katriel ]

## [03453] Optimal vaccination at high reproductive numbers: sharp transitions and counter-intuitive allocations

**Format :** Talk at Waseda University

**Author(s) :** Nir Gavish (Technion - Israeli Institute of Technology)Guy Katriel (Braude College of Engineering)

**Abstract :** Optimizing vaccine allocation is crucial for effective vaccination campaigns against epidemics. Contrary to intuition and classic vaccination theory, we show that for leaky vaccines and high basic reproduction numbers, the optimal allocation strategy for minimizing infections prioritizes those least likely to be infected. These findings have important implications for managing vaccination campaigns against highly transmissible infections.

## [04794] An epidemic model for reinfection dynamics with heterogeneous susceptibility

**Format :** Talk at Waseda University

**Author(s) :** Yukihiko Nakata (Aoyama Gakuin University)

**Abstract :** Individuals in a population vary in susceptibility. To explore the impact of the distributed susceptibility, we consider an epidemic model, where individuals acquire a degree of susceptibility with a probability after infection. It is shown that heterogeneous susceptibility adds complexity to the reinfection dynamics, and changes in the distribution of susceptibility may cause unexpected epidemics. We revisit the epidemic model studied by Katriel in 2010. The study is partly a joint work with Ryosuke Omori.

## [03972] Effective screening with rapid antigen tests for COVID-19 patients: simulation with viral dynamics model

**Format :** Talk at Waseda University

**Author(s) :** Yong Dam Jeong (Nagoya University)Keisuke Ejima (Nanyang Technological University)Ajelli Marco (Indiana University School of Public Health-Bloomington)Shingo Iwami (Nagoya University)

**Abstract :** In this study, we assessed the effectiveness of various screening strategies with rapid antigen tests in schools and workplaces. For this, we developed two models with different scales: a transmission model in the community where those facilities under screening tests belong, and a viral dynamics model of each infected case in those facilities. Those screening strategies were compared through quantitative simulations. Our computational framework will be useful to evaluate screening strategies for infectious disease transmission.

## [03510] Evaluation of Effectiveness of Global COVID-19 Vaccination Campaign in 2021

**Format :** Talk at Waseda University

**Author(s) :** Daihai He (Hong Kong Polytechnic University)

**Abstract :** To model estimated deaths averted by COVID-19 vaccines, we used state-of-the-art mathematical modeling, likelihood-based inference, and reported COVID-19 death and vaccination data. We estimated that >1.5 million deaths were averted in 12 countries. Our model can help assess effectiveness of the vaccination program, which is crucial for curbing the COVID-19 pandemic.

02491 (2/2) : 4E @A201 [Chair: Yukihiko Nakata]

## [03458] Exploring the dynamics of contagion models with stages

**Format :** Talk at Waseda University

**Author(s) :** Guy Katriel (Braude College of Engineering)

**Abstract :** We study models which are similar to classical epidemiological models, but in which becoming 'contagion' involves a process with several stages. Such mechanisms are natural when considering phenomena of 'social contagion' - the transmission of beliefs, behaviors. It is shown that these models display a variety of nonlinear behaviors that are absent in the corresponding 'classical' epidemiological models, including: bistability, critical transitions, endogenous oscillations, and excitability. These phenomena, and the bifurcations involved, are studied by a combination of analytical and numerical means. We thus suggest that two-stage (or multi-stage) contagion can serve as a possible explanatory mechanism for some of the complex dynamical phenomena observed in social life.

## [04574] Mathematical modeling of COVID-19 transmission with pandemic response in South Korea

**Format :** Talk at Waseda University

**Author(s) :** Yongin Choi (National Institute for Mathematical Sciences)Kyeongah Nah (National Institute for Mathematical Sciences)

**Abstract :** In this study, we investigated the effects of control policies on the COVID-19 outbreak in South Korea using a transmission dynamics model, where its transmission rate is estimated by a machine-learning algorithm. Our findings showed that the effectiveness of these policies varied across different waves of the epidemic and was influenced by various factors, such as vaccination coverage and mobility levels. Our findings emphasize the importance of a data-driven approach to evaluate COVID-19 policies.

## [03885] Front propagation in an epidemiological model with mutations

**Format :** Talk at Waseda University

**Author(s) :** Hiroshi Matano (Meiji University)Quentin Griette (Université Le Havre Normandie)

**Abstract :** We consider a reaction-diffusion system describing the propagation of disease that involves mutation of the pathogen. More precisely this is an S-I-S epidemic model with diffusion in which two types of pathogens appear (wild and mutant). We assume that mutation occurs reciprocally between the two types at a certain rate. The resulting reaction-diffusion system has a peculiar feature: it is of the cooperative nature for small density of infected population while it is of the competitive nature for large density. This model was introduced by Q.Griette and G.Raoul in 2016 for a spatially homogeneous environment. Similar systems were also studied slightly later by L.Girardin and by E.Crooks et al, also for the spatially homogeneous case.

In this talk, I will consider this system in spatially periodic environments and present the following results: (1) existence of traveling waves; (2) spreading speed of infection when starting from localized initial data; (3) stability and asymptotic profile of propagating fronts. I will also discuss the homogenization limit of the problem when the spatial period of the environment tends

## [05100] Resolving the enigma of COVID-19 outbreaks in Iquitos and Manaus

**Format :** Talk at Waseda University

**Author(s) :** lewi stone (RMIT University)Daihai He (Hong Kong Polytechnic University)

**Abstract :** The nearby cities of Iquitos (Peru) and Manaus (Brazil) experienced the world's highest infection and mortality rates

during the first 2020 COVID-19 wave. Key studies suggested >70% of the Manaus population was infected, and thus

close to herd immunity and protected. It remains an enigma as to why a deadly second wave followed in Manaus. We

present a data-driven model of epidemic dynamics in Iquitos to help explain and model events in Manaus

## [02493] Advanced Modelling of Complex Nonlinear Systems

**Session Time & Room :** 4E (Aug.24, 17:40-19:20) @G704

**Type :** Proposal of Minisymposium

**Abstract :** Complex nonlinear systems with millions and even billions of parameters appear in various fields of science and engineering. These include mechanics, fluid dynamics, and deep neural networks. In order to better understand, predict and optimize the solutions, new mathematical models are required.

In this mini-symposium, we plan to present several approaches from different fields related to modeling large high-dimensional nonlinear systems. This will foster better synergy and collaboration of researchers from various disciplines. Researchers from advanced signal processing, applied mathematics, and fluid mechanics will discuss their contributions. We anticipate new insights and analogies will be gained following this exchange of ideas.

**Organizer(s) :** Ido Cohen, Guy Gilboa

**Classification :** 37-00, 35-00, 49-00, 76-00

**Minisymposium Program :**

part\_2

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02493 (1/1) : 4E @G704

## [03289] A Minimal Set of Koopman Eigenfunctions -- Analysis and Numerics

**Author(s)** : Ido Cohen (Technion - Israel Institute of Technology)

**Abstract** : In this talk, we present the most concise linear representation of nonlinear systems based on the theory of Koopman Operator. Here, we define the “basis” of Koopman eigenfunctions from which the whole spectrum of the Koopman operator can be generated and the dynamic is accurately reconstructed. Numerically, the curse of dimensionality in samples vanishes since the inherent geometry constraints. Thus, the suggested method yields the most reduced representation from samples justifying the term *minimal set*.

## [03525] Acoustic Streaming

**Author(s)** : James Friend (University of California San Diego)

**Abstract** : Acoustic streaming is a nonlinear effect from an acoustic wave that can generate rapid fluid flows. We show a new, mathematically challenging approach to its analysis that overcomes past limitations, recasting traditional separation of scales in one variable to separation of spatiotemporal scales, with careful treatment of partial derivatives and the definition of compatibility equations to ensure closure. We provide closed-form solutions to transient acoustic streaming for the first time.

## [04735] The Underlying Correlated Dynamics in Neural Training

**Author(s)** : Guy Gilboa (Technion)Rotem Turjeman (Technion)Tom Berkov (Technion)Ido Cohen (Technion)

**Abstract** : We propose a model of neural-net training which dramatically reduces the dimensionality. Our algorithm, Correlation Mode Decomposition (CMD), yields groups of highly correlated parameters. We achieve a remarkable dimensionality reduction with this approach, where a network of 11M parameters like ResNet-18 can be modeled well using just a few modes. Retraining the network using our model induces a regularization which yields better generalization capacity on the test set.

## [05114] A Nonstochastic Control Approach to Optimization

**Author(s)** : Xinyi Chen (Princeton University and Google AI)Elad Hazan (Princeton University and Google AI)

**Abstract** : Selecting the best hyperparameters, such as the learning rate and momentum, is an important but nonconvex problem. We propose an online nonstochastic control methodology for optimization that can circumvent this nonconvexity and obtain certain global guarantees. The problem of learning the best optimizer can be framed as a feedback control problem over the choice of optimizers. Our method guarantees that we can compete with the best optimizer in hindsight from a class of methods on a given sequence of problems.

# [02499] Machine Learning for dynamics and its applications

**Session Time & Room :**

02499 (1/4) : 3C (Aug.23, 13:20-15:00) @F308

02499 (2/4) : 3D (Aug.23, 15:30-17:10) @F308

02499 (3/4) : 3E (Aug.23, 17:40-19:20) @F308

02499 (4/4) : 4C (Aug.24, 13:20-15:00) @F308

**Type** : Proposal of Minisymposium

**Abstract** : There has been a growing interest in exploiting machine learning to predict the behaviors of complex nonlinear dynamics. It is also of interest to clarify to what extent machine learning can be used to model and predict dynamical system structures that do not appear in training time series explicitly. In this mini-symposium, we will learn of new results on machine learning for dynamics and its applications to complex phenomena such as fluid and climate dynamics. Examples include the prediction of invariant sets (fixed points, periodic points, strange attractors, and invariant manifolds) and their stabilities, tipping point, and missing dynamics.

part\_2

**Organizer(s)** : Masanobu Inubushi, Kengo Nakai, Hirofumi Notsu, Yoshitaka Saiki

**Classification** : 37Nxx, Machine learning, Reservoir computing, Data-driven modeling, Dynamical systems

**Minisymposium Program :**

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02499 (1/4) : 3C @F308 [Chair: Hirofumi Notsu]

## [04040] Construction of differential equations from scalar chaotic time series

**Format** : Talk at Waseda University

**Author(s)** : NATSUKI TSUTSUMI (Hitotsubashi University)kengo nakai (Okayama University)Yoshitaka Saiki (Hitotsubashi University)

**Abstract** : We propose a method of constructing a system of differential equations of chaotic behavior only from observable scalar time series. The method employs a regression using Gaussian radial basis functions together with polynomial terms. We apply it to several chaotic time series. The obtained model is assessed from the viewpoint of time series forecast, reconstruction of invariant sets, and invariant densities. Delay coordinate and a chaotic saddle have played a big role in the procedure.

## [04709] Data-driven inference of Navier-Stokes turbulence from limited observations

**Format** : Talk at Waseda University

**Author(s)** : Masanobu Inubushi (Tokyo University of Science)

**Abstract** : Inference of turbulent states governed by the Navier-Stokes equations is one of the challenging and crucial problems for applied mathematics and industrial applications because of the high dimensionality and nonlinearity of fluid dynamics. In this study, we propose a data-driven inference method of turbulent dynamics from limited observations, which is suitable for industrial applications, and discuss its performance from the viewpoint of dynamical system theory.

## [03862] Long-lead prediction of Indian Summer Monsoon onset with reservoir computing

**Format** : Talk at Waseda University

**Author(s)** : Takahito Mitsui (Technical University of Munich)Niklas Boers (Technical University of Munich)

**Abstract** : Although the prediction of the Indian Summer Monsoon (ISM) onset is of crucial importance for water-resource management and agricultural planning on the Indian sub-continent, the long-term predictability, especially at seasonal time scales, is little explored. We propose a method based on reservoir computing that provides skilful long-term forecasts of the ISM onset. Our study demonstrates that machine-learning-based approaches can be simultaneously helpful for both data-driven prediction and enhancing the process understanding of climate phenomena.

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02499 (2/4) : 3D @F308 [Chair: Yoshitaka Saiki]

## [03000] Learning Strange Attractors with Reservoir Systems

**Format** : Talk at Waseda University

**Author(s)** : Allen Hart (University of Bath)

**Abstract** : This talk is based on a preprint by myself, Juan-Pablo Ortega, and Lyudmila Grigoryeva, which shows that the celebrated Takens Embedding Theorem is a particular case of a much more general statement according to which, randomly generated Echo State Networks (with linear activations) trained on generic observations of an invertible dynamical system carry in their wake an embedding of the phase space dynamics into the chosen Euclidean state space. This embedding coincides with a natural generalized synchronization that arises in this setup and that yields a topological conjugacy between the state-space dynamics driven by the generic observations of the dynamical system and the dynamical system itself. This result provides additional tools for the representation, learning, and analysis of chaotic attractors and sheds additional light on the reservoir computing phenomenon that appears in the context of recurrent neural networks.

## [04147] Dynamical system properties of reservoir computing models

**Format :** Talk at Waseda University

**Author(s) :** kengo nakai (Okayama University)Miki U. Kobayashi ( Risho University)Yoshitaka Saiki (Hitotsubashi University)Natsuki Tsutsumi (Tokyo University of Marine Science and Technology)

**Abstract :** It has been reported that reservoir computing is effective in the inference of time-series and some characteristics. We construct a model from training time-series of dynamical system with tangencies between stable and unstable manifolds or hetero-chaos, coexisting of invariant sets of different number of unstable dimensions. We confirm that these dynamical properties as well as fixed points and periodic orbits can be reconstructed by reservoir computing.

## [02889] Predicting tipping point with machine learning

**Format :** Talk at Waseda University

**Author(s) :** Ying-Cheng Lai (Arizona State University)

**Abstract :** Compared with the existing works on model-free prediction of chaotic systems, to predict a tipping point is significantly more challenging, because the training data are from the system when it is in a steady state. The speaker will describe the tipping-point mechanism, discuss how dynamical noise can be exploited in a machine learning scheme to predict the future occurrence of tipping points, and present benchmark examples as well as a real-world application.

## [02921] Machine Learning for Predicting Missing Dynamics

**Format :** Talk at Waseda University

**Author(s) :** Shixiao Willing Jiang (ShanghaiTech University)

**Abstract :** We present a framework for recovering missing dynamics using available data and machine learning techniques. The framework reformulates the prediction problem as a supervised learning problem to approximate a map that takes the memories of the resolved and identifiable unresolved variables to the missing components in the resolved dynamics. The map for this non-Markovian transition kernel is represented by appropriate RKHS or LSTM formulation. Supporting numerical results include the Lorenz system, the Kuramoto-Sivashinsky equation, etc.

02499 (3/4) : 3E @F308 [Chair: Kengo Nakai]

## [05374] Kernel Flows and Kernel Mode Decomposition for Learning Dynamical Systems from Data

**Format :** Talk at Waseda University

**Author(s) :** Boumediene Hamzi (Caltech)

**Abstract :** Regressing the vector field of a dynamical system from a finite number of observed states is a natural way to learn surrogate models for such systems. We present variants of the method of Kernel Flows as simple approaches for learning the kernel that appear in the emulators we use in our work. First, we will talk about the method of parametric and nonparametric kernel flows for learning chaotic dynamical systems. We'll also talk about learning dynamical systems from irregularly-sampled time series as well as from partial observations. We will also introduce the method of Sparse Kernel Flows and apply it to learn 132 chaotic dynamical systems. Finally, we extend the method of Kernel Mode Decomposition to design kernels in view of detecting critical transitions in some fast-slow random dynamical systems.

This is joint work with Yang Lu, Xiuwen Sun, Houman Owhadi, Leo Paillet, Naiming Xie

## [05420] Discovery of quasiperiodically driven dynamics using kernel methods

**Format :** Talk at Waseda University

**Author(s) :** Sudhasattwa Das (Texas Tech University)Shaurya Agarwal (University of Central Florida)Shakib Mustavee (University of Central Florida)

**Abstract :** Quasiperiodically driven dynamical systems are nonlinear systems which are driven by some periodic source with multiple base-frequencies. Such systems abound in nature, and are present in data collected from sources such as astronomy and traffic data. Such dynamics decomposes into two components - the driving quasiperiodic source with generating frequencies; and the driven nonlinear dynamics. Analysis of the quasiperiodic part presents the same challenges as classical Harmonic analysis. On the other hand, the nonlinear part bears all the aspects of chaotic dynamics, and possibly carry stochastic perturbations. We present a kernel-

part\_2

based method which provides a robust means to learn both these components. It uses a combination of a kernel based Harmonic analysis and kernel based interpolation technique, to discover these two parts. The technique performs reliably in several real world systems, ranging from analyzing the human heart to traffic data.

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02499 (4/4) : 4C @F308 [Chair: Masanobu Inubushi]

## [05427] Reservoir Computing Generalized

**Format :** Talk at Waseda University

**Author(s) :** Tomoyuki Kubota (The University of Tokyo)

**Abstract :** Reservoir computing (RC) is a machine learning framework that leverages a dynamical system as an information processor. This framework imposes a constraint on a system where the system must exhibit an identical response against an identical input sequence to work as a reproducible input processor; however, systems that violate the constraint can also process input. In this talk, we introduce a more general theoretical framework called generalized reservoir computing, covering the rest of irreproducible systems.

## [05429] Reservoir computing with the Kuramoto model

**Format :** Talk at Waseda University

**Author(s) :** Koichi Taniguchi (Tohoku University)

**Abstract :** The physical reservoir aims to achieve high-performance and low-cost machine learning by using real physical systems as reservoirs, but in general, there is no theoretical guideline for high-performance or optimality. In this talk, we discuss the reservoir computing with the Kuramoto model and the "edge of bifurcation" conjecture which means that its best performance is achieved by taking the model parameters just below the bifurcation point of the dynamical system.

## [05431] Embedding bifurcation structures into a soft robotic actuator

**Format :** Talk at Waseda University

**Author(s) :** Nozomi Akashi (Kyoto University)Yasuo Kuniyoshi (The University of Tokyo)Taketomo Jo (Bridgestone Corporation)Mitsuhiko Nishida (Bridgestone Corporation)Ryo Sakurai (Bridgestone Corporation)Yasumichi Wakao (Bridgestone Corporation)Kohei Nakajima (The University of Tokyo)

**Abstract :** We demonstrate that bifurcation structures can be embedded into a McKibben pneumatic artificial muscle, which is a common soft robotic actuator, through closed-loop control of physical reservoir computing. Our experiments reveal that both periodic and chaotic dynamics can be embedded into the artificial muscle by training only one side of these dynamics. Our results provide insight into reducing the amount and types of training data required for robot control through the utilization of bifurcation structures.

## [05402] Physical reservoir computing using dynamics of biological neuronal network with modular structure

**Format :** Talk at Waseda University

**Author(s) :** Takuma Sumi (Tohoku University)Hideaki Yamamoto (Tohoku University)Yuichi Katori (Future University of Hakodate)Koki Ito (Tohoku University)Shigeo Sato (Tohoku University)Ayumi Hirano-Iwata (Tohoku University)

**Abstract :** Physical reservoir computing with biological neuronal network (BNN) has recently advanced the understanding of its computational principles. However, the BNN in conventional culture was randomly connected, generating non-physiological dynamics. Here, we employed micropatterning technology to fabricate BNNs with modular topology conserved evolutionarily in animal brains. We showed that the BNN reservoir exhibited higher classification when its network was functionally modular. Our findings provide insights into the link among non-random network connectivity, neuronal dynamics, and computing.

# [02514] Developing Performance Portable, Scalable and AI enabled Fusion Energy Physics Framework

## **Session Time & Room :**

02514 (1/2) : 5C (Aug.25, 13:20-15:00) @E606

02514 (2/2) : 5D (Aug.25, 15:30-17:10) @E606

## **Type :** Proposal of Minisymposium

**Abstract :** The plasma physics and tokomak engineering are widely recognized as a challenging "exascale" multi-scale multi-physics application. Recent advances in exascale computing, artificial intelligence (AI), and machine learning have paved the way for unprecedented opportunities in "in-silico" fusion reactor interpretation and design. Deep learning and the availability of powerful, easy-to-use HPC/ML toolboxes have played a significant role in achieving such breakthroughs. In this minisymposia, we are aiming to present recent advances in general numerical methods with adaptive meshes, AI methods, surrogate modelling, and performance-portable programming techniques for current and future computing architectures.

**Organizer(s) :** Xiaohu Guo, Jony Castagna, Vignesh Gopakumar, Stanislas Pamela

**Classification :** 65M25, 68T07, 35Q83, 65M50, 68Q85

## **Minisymposium Program :**

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02514 (1/2) : 5C @E606

## [04465] Develop next generation CFD tools using AI libraries

### **Author(s) :** Xiaohu Guo (UKRI STFC Hartree Centre)

**Abstract :** Due to new hardware technologies, increases in computing power and developments in AI software, the benefits of combining AI techniques with traditional numerical methods for solving governing equations of dynamical systems are becoming apparent. This talk introduces a revolutionary approach to the discretization and solution of PDEs. Our approach implements CFD models using neural network with the aim of simplifying the software development and building on the very substantial developments already made in AI software.

## [04466] Cheap training sets of gyrokinetic surrogate models with active learning

### **Author(s) :** Xiaohu Guo (UKRI STFC Hartree Centre)Lorenzo Zanisi (UKAEA)

**Abstract :** Surrogate models of gyrokinetic turbulence play critical role in accelerating integrated models thus leading to faster post-discharge analysis, operations optimisation and flight simulator applications. Training sets for surrogates are obtained by brute-force approaches which may cause unnecessary, expensive oversampling, which limits the dimensionality of the input space and applications to high fidelity codes. We develop two-stage Active Learning pipeline to efficiently sample the input parameter space of gyrokinetic models, benchmark applications in multichannel integrated models.

## [04627] Implementation of a finite element PDE solver in AMReX

### **Author(s) :** Karthikeyan Chockalingam (UKRI STFC Hartree Centre)Alex Grant (UKRI STFC Hartree Centre)Xiaohu Guo (UKRI STFC Hartree Centre)

#### **Abstract :**

The scope of the current work is to embed a finite element implementation in AMReX. One of the advantages of using block-structured meshes is that each element does not require a unique isoparametric mapping. Initial testing of the implementation on the Poisson problem shows considerable performance gain compared to an unstructured finite element framework. The framework allows for the ease of implementing different types of higher-order elements. It has also been extended for solving Navier-Stokes.

## [04652] AI deconvolution operator for plasma turbulent simulations on complex geometries

**Author(s)** : Jony Castagna (UKRI-STFC Hartree Centre)Francesca Schiavello (UKRI-STFC Hartree Centre)

**Abstract** : We use Generative Adversarial Networks (GANs) to model the nonlinear terms in partial differential equations on coarse structured grids. The idea is to reconstruct the high-resolution fields exploring the latent space of the GANs after being properly trained on curvilinear coordinates. The nonlinear terms are then found and mapped back to the coarse structured mesh where the filtered equations are solved. Results for Navier Stokes and Hasagawa-Wakatani plasma equations are presented.

02514 (2/2) : 5D @E606

## [04741] Performance and scaling of amrPX: a multiphase CFD framework

**Author(s)** : Alex Grant (UKRI STFC Hartree Centre)Xiaohu Guo (UKRI STFC Hartree Centre)Karthikeyan Chockalingam (UKRI STFC Hartree Centre)

**Abstract** : amrPX is a modularised, multi-model adaptive mesh refinement framework built using AMReX. Each model has a common structure with Data, Solver, Physics and Problem containers, with shared utility modules such as numerics or materials, to promote code re-use and ease of development. A compressible multiphase Five-Equation model has been implemented and benchmarked. Performance results and scalability across thousands of CPUs and GPUs is discussed.

## [05229] A highly parallel simulation of patient-specific hepatic flows

**Author(s)** : Zeng Lin (Shenzhen Institute of Advanced Technology, Chinese Academy of Sciences)

**Abstract** : Computational hemodynamics is being developed as an alternative approach for assisting clinical diagnosis and treatment planning for liver diseases. The technology is non-invasive, but the computational time could be high when the full geometry of the blood vessels is taken into account. In this work, we study a highly parallel method for the transient incompressible Navier-Stokes equations for the simulation of the blood flows in the full three-dimensional patient-specific hepatic artery, portal vein and hepatic vein. As applications, we also simulate the flow in a patient with hepatectomy and calculate the portal pressure gradient. One of the advantages of simulating blood flows in all hepatic vessels is that it provides a direct estimate of the portal pressure gradient, which is a gold standard value to assess the portal hypertension. Moreover, the robustness and scalability of the algorithm are also investigated. A 83% parallel efficiency is achieved for solving a problem with 7 million elements on a supercomputer with more than 1000 processor cores.

## [02515] Novel deep learning methodologies in Industrial and Applied Mathematics

**Session Time & Room :**

02515 (1/2) : 5B (Aug.25, 10:40-12:20) @E818

02515 (2/2) : 5C (Aug.25, 13:20-15:00) @E818

**Type** : Proposal of Minisymposium

**Abstract** : The proposed mini-symposium is focused on a few novel techniques in IAM, their applications and promising opportunities. The techniques considered rely on artificial intelligence methods to solve problems in engineering, like wind turbine preventive maintenance or predicting molecular weights of industrial polymers using diffusion NMR spectroscopy; to advance in making AI more reliable by enabling it to cope with causality and thereby enhancing its explainability; to promote neural networks capable of directly processing geometric entities and use them for robust deep learning in various domains, including artificial vision; and to tackle with the engineering problems of multiphasic electric power generation.

**Organizer(s)** : Sebastian Xambó-Descamps, Yolanda Vidal, Eduardo U. Moya Sánchez

**Classification** : 68Txx, 78A25, 78A40, 78A57, 70-XX, 68T07, 68T27, 68T45; 70-08, 70-10

**Minisymposium Program :**

02515 (1/2) : 5B @E818 [Chair: Marta Barroso]

## [05353] Artificial Intelligence for Wind Turbine Predictive Maintenance

**Format :** Online Talk on Zoom

**Author(s) :** Yolanda Vidal (Universitat Politècnica de Catalunya. Jordi Girona 31. 08034. Barcelona. VAT: ESQ0818003F)

**Abstract :** This proposal states a data-driven predictive maintenance (PM) strategy for wind turbines that uses artificial neural networks with Bayesian regularization and Levenberg-Marquardt optimization. The proposed strategy aims to address challenges associated with SCADA data such as high dimensionality, low sampling rate, and unbalanced datasets. The strategy will be validated on real SCADA data from a wind farm consisting of 12 wind turbines and is expected to provide reliable predictions with minimum false alarms and early warnings months in advance. This PM approach can help reduce the levelized cost of energy (LCOE) of wind farms and promote renewable energy as a cost-effective solution to achieve energy independence and combat climate change.

## [03575] Innovative Models for Explainable Artificial Intelligence

**Format :** Online Talk on Zoom

**Author(s) :** Silvia Franchini (National Research Council of Italy)Francesco Prinzi (University of Palermo)Salvatore Vitabile (University of Palermo)

**Abstract :** Traditional data-driven ML approaches show very interesting performance even if their internal mechanisms are very cryptic (black box). However, in some critical contexts, model interpretability is mandatory to explain the learned functionality, becoming even a legal requirement. Among the benefits of reformulating neural networks through the geometric calculus paradigm, geometric interpretability could potentially serve as a characteristic that improves model transparency. This work proposes the use of higher-dimensional neurons to reduce computational complexity while preserving model accuracy.

## [05376] Applications of Quaternion Monogenic Signal ConvNet Layer

**Format :** Online Talk on Zoom

**Author(s) :** E. Ulises Moya-Sanchez (Universidad Autonoma de Guadalajara/Gobierno de Jalisco)Genaro Paredes (Universidad Autonoma de Guadalajara)Sebastian Xambó-Descamps (UPC)Ulises Cortes (BSC)Abraham Sanchez (Gobierno de Jalisco)

**Abstract :** The monogenic ConvNet layer is a quaternion bio-inspired input layer. This layer creates a new geometric feature space using the Fourier transform. This new representation assigns a structural and geometrical interpretation to each image point and allows the detection of local symmetry elements (such as line-like or edge-like). Its main strength is that it behaves robustly under a variety of illumination transforms. In this work we present the design details and characteristics of this layer and consider a number of situations in which it can be applied.

## [05352] Novel deep learning methodologies in Industrial and Applied Mathematics

**Format :** Online Talk on Zoom

**Author(s) :** Sebastian Xambó-Descamps (IMTech and BSC)

**Abstract :** This talk, with the same title as the MS, is meant to be the first and it aims at a broad presentation of the most promising novel methodologies in IAM based on deep learning techniques, with a particular attention focused on those pioneered by the MS speakers.

02515 (2/2) : 5C @E818 [Chair: Marta Barroso]

## [05354] AI Lifecycle Zero-touch Orchestration within the Edge-to-Cloud Continuum for Industry 5.0

**Format :** Talk at Waseda University

**Author(s) :** Marta Barroso Barroso (Barcelona Supercomputing Center)

**Abstract :** AI is one of the biggest megatrends towards the 5th industrial revolution. Although these technologies promise business sustainability as well as product and process quality, it seems that the ever-changing market demands and the complexity of technologies, impede broad application and reuse of Artificial intelligence (AI) models across the industry. KnowlEdge is an European project funded by the Horizon 2020 (H2020) that aims to develop of a new generation of AI methods, systems, and data management infrastructure in order to break the entry barriers for these technologies and unleash its full potential. In particular, knowlEdge project converges techniques from part\_2

multiple computing areas, including AI , distributed data analytics, IoT, software engineering, edge and Cloud technologies into a unified software architecture. The outcomes of the project not only enable the automated extraction and utilization of data coming from multiple and geographically dispersed sources, it also provides a way of reusing and sharing AI models in an (semi-)automated way in particular companies that are only able to perform the execution of models rather than the training themselves.

## [02526] Recent Developments of Mathematical Economics Focusing on Macroeconomic Dynamics

**Session Time & Room :** 5D (Aug.25, 15:30-17:10) @D502

**Type :** Proposal of Minisymposium

**Abstract :** Successful investigation is highlighted about application of cutting-edge mathematical methodology to traditional macroeconomic models. We will show how modern methodology can fit into these studies. In particular, the session presents an evaluation of a deterministic limit cycle in a stochastic post-Keynesian model, endogenous fluctuations of money and foreign exchange ratio in a Mundell-Fleming international trade framework, applications of nonlinear differential equations for the birth of GDP fluctuations in a three-country Kaldor model with fixed exchange rates and estimation of the natural rate of interest by utilizing various filters, which is one of the significant topics of empirical macroeconomics

**Organizer(s) :** Akio Matsumoto, Ferenc Szidarovszky

**Classification :** 91B55, 91-05, 91-10, 62P20

**Minisymposium Program :**

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02526 (1/1) : 5D @D502 [Chair: Akio Matsumoto]

### [04358] On growth cycles in a stochastic post-Keynesian model

**Format :** Talk at Waseda University

**Author(s) :** Hiroki Murakami (Chuo University)

**Abstract :** This study evaluates the impact of stochastic disturbances on a deterministic limit cycle in a stochastic post-Keynesian model. It presents an approximation formula for solution paths near the limit cycle and derives an approximated distribution of the limit cycle.

### [03425] A Three-Country Kaldorian Business Cycle Model with Fixed Exchange Rates

**Format :** Talk at Waseda University

**Author(s) :** Toichiro Asada (Faculty of Economics, Chuo University)

**Abstract :** This paper analyzes a three-country, fixed exchange rates Kaldorian nonlinear macrodynamic model of business cycle. The country is connected through international trade, and international capital movement with imperfect capital market. Our model is a continuous time version that is formulated by a eight-dimensional nonlinear differential equations. This system is studied both analytically and numerically. This paper is a joint work by R. Zimka, M. Demetrian, T. Asada, and T. Inaba.

### [04424] Simple Estimations of the Natural Rate of Interest

**Format :** Talk at Waseda University

**Author(s) :** Kazuhiko NAKAHIRA (Meikai University)

**Abstract :** The natural rate of interest is an important concept since it is a kind of reference for a variety of policy rules to characterize our monetary policy. One of the simple ways of estimating the natural rate of interest is to extract the trend of the real short-term interest rate. We utilize the Hodrick-Prescott filter, the Baxter-King filter, and the Christiano-Fitzgerald filter for our extraction. In addition, we have an inference of expected inflation rate.

## [04486] Dynamic Adjustment in the Mundell-Fleming Model

**Format :** Online Talk on Zoom

**Author(s) :** Hiroyuki Yoshida (Nihon University)

**Abstract :** The purpose of this presentation is to show the emergence of perpetual and endogenous fluctuations in the global economy by using the Hopf bifurcation theorem. The model we consider is the dynamic version of the Mundell-Fleming model, which deals with the short-run relationship between output, interest rate, and foreign exchange rate in a small open economy. We show that the steady state is locally stable when the adjustment speed of the foreign exchange market is sufficiently slow.

## [02527] AI for Healthcare and Medicine

**Session Time & Room :**

02527 (1/2) : 1D (Aug.21, 15:30-17:10) @E604

02527 (2/2) : 1E (Aug.21, 17:40-19:20) @E604

**Type :** Proposal of Minisymposium

**Abstract :** The minisymposium will explore the various ways in which artificial intelligence is being used in the field of healthcare and medicine, with a focus on the use of privacy-preserving machine learning. The symposium will feature presentations from experts in the field, who will discuss the latest developments and trends in AI for healthcare and medicine, including the use of federated learning and data collaboration for training machine learning models on decentralized data. The symposium will provide attendees with a comprehensive overview of the current state of AI in healthcare and medicine, and will offer insights into the potential future developments in this rapidly evolving

**Organizer(s) :** Tetsuya Sakurai, Akira Imakura, Weichung Wang, Li-Chen Fu

**Classification :** 65Fxx, 92Fxx

**Minisymposium Program :**

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02527 (1/2) : 1D @E604 [Chair: Weichung Wang]

## [02894] Data Collaboration Cox Proportional Hazards Model for Privacy-preserving Survival Analysis

**Format :** Talk at Waseda University

**Author(s) :** Akira Imakura (University of Tsukuba)Ryoya Tsunoda (University of Tsukuba Hospital)Rina Kagawa (University of Tsukuba)Kunihiro Yamagata (University of Tsukuba)Tetsuya Sakurai (University of Tsukuba)

**Abstract :** In recent years, privacy-preserving machine learning for datasets held by multiple organizations in a distributed manner has been attracted attention. In this study, we focus on privacy-preserving survival analysis for datasets held by multiple medical institutions and propose a data collaboration technique that shares dimensionality-reduced intermediate representations instead of raw data. The proposed DC-COX can calculate the contribution of each feature to survival time and the corresponding p-value. Numerical experiments verify the effectiveness of DC-COX.

## [05307] AI-Enhanced Medical Imaging Analysis: Advancing Precision Treatment for NSCLC Brain Metastases

**Format :** Talk at Waseda University

**Author(s) :** Cheyu Hsu (National Taiwan University Hospital)

**Abstract :** In this talk, we discuss the innovative use of radiomics and deep learning in AI-enhanced medical imaging analysis for managing NSCLC brain metastases. Through automated segmentation, we streamline diagnosis and treatment planning. The presentation delves into predicting local recurrence after radiosurgery, detecting EGFR mutations, and evaluating distant metastases or brain metastases velocity in radiosurgery-treated patients. Our focus on AI-driven methodologies fosters tailored, precision treatment strategies, ultimately enhancing patient outcomes for those with NSCLC brain metastases.

## [05001] Explainability and Fairness of Distributed Data Analysis

**Format :** Talk at Waseda University

**Author(s) :** Anna Bogdanova (University of Tsukuba)Tetsuya Sakurai (University of Tsukuba)Akira Imakura (University of Tsukuba)

**Abstract :** Ensuring fairness and transparency in machine learning models is critical for their ethical application in the medical field. With the increasing use of distributed machine learning to protect patient privacy, there is a growing need to address the challenges of explainability and fairness in medical data analysis. Machine learning models trained on horizontally or vertically partitioned medical data may present difficulties for explainability, as different participants may have a biased view of the background data or a partial view of the feature space, leading to inconsistencies in the explanations obtained. To address these issues, this paper proposes an Explainable Data Collaboration Framework that combines a model-agnostic additive feature attribution algorithm (KernelSHAP) with a privacy-preserving distributed machine learning method called Data Collaboration. The framework offers three algorithms for various scenarios of explainability in medical data collaboration, which were tested on open-access medical datasets. In addition, we show that our proposed framework can be combined with fairness-sensitive data representation techniques to eliminate data biases at the local level.

## [05362] Mitigating Non-IID Data Challenges in Federated Learning for Healthcare Applications

**Format :** Talk at Waseda University

**Author(s) :** Fan Zhang (University of Cambridge)

**Abstract :** Federated Learning has emerged as a promising technique for healthcare applications, enabling collaboration among different healthcare institutions without sharing sensitive data. Data in each healthcare institution usually has a unique distribution, leading to non-IID (independent and identically distributed) data that can impact model performance and convergence in Federated Learning. In this talk, we will present the findings of non-IID challenges in Federated Learning and recommendations for the strategies we evaluated to mitigate these challenges.

02527 (2/2) : 1E @E604 [Chair: Akira Imakura]

## [03888] Causal inference and machine learning on distributed data

**Format :** Talk at Waseda University

**Author(s) :** Yuji Kawamata (Center for Artificial Intelligence Research, University of Tsukuba)Ryoki Motai (Graduate School of Science and Technology, University of Tsukuba)Yukihiko Okada (Center for Artificial Intelligence Research, University of Tsukuba)Akira Imakura (Center for Artificial Intelligence Research, University of Tsukuba)Tetsuya Sakurai (Center for Artificial Intelligence Research, University of Tsukuba)

**Abstract :** Utilizing distributed data allows for more reliable estimation of conditional average treatment effects. However, it is difficult to share data owing to privacy concerns. To address this issue, we proposed Data Collaboration Double Machine Learning (DC-DML), which can address horizontally and vertically distributed data and provide point and interval estimation. In experiments using synthetic data, we found that DC-DML could lead to more accurate estimation results than when using distributed data individually.

## [05313] Precision Preventive Medicine in Sub-Healthy Population

**Format :** Talk at Waseda University

**Author(s) :** Han-Mo Chiu (National Taiwan University Hospital)Hung-Ju Lin (National Taiwan University Hospital)

**Abstract :** Preventing the onset or progression of non-communicable diseases in sub-health population tremendously impact the population health and the related cost and both primary and secondary prevention play pivotal roles in this aspect. The State-of-the-art digital health and artificial intelligence technologies have been applied widely in the healthcare sector, and are anticipated to play a more proactive role in preventive medicine in terms of risk stratification, adopting clinical, genomic, or metagenomic information, and leveraging lifestyle modification.

## [03660] Medical AI, Biosensors and Privacy

**Format :** Talk at Waseda University

**Author(s) :** Takeshi Kimura (University of Tsukuba)

**Abstract :** As Medical AI is expected to improve health care, there is also a concern regarding collecting personal data via AI devices, including biosensors. Advanced biosensors could read and collect inner physiological, emotional, and sensitive conditions. However, patients cannot control their private information collected with biosensors and, once they become data belonging to a hospital or data collection company, cannot have access to their private information. The associated ethical issues are examined.

## [05312] HeortaNet: AI for Quantifying Heart Structures on Non-Contrast CT Images

**Format :** Talk at Waseda University

**Author(s) :** Wen-Jeng Lee (Department of Medical Imaging, National Taiwan University Hospital)

**Abstract :** HeortaNet is an AI model developed by TW-CVAI for the segmentation of pericardium/aorta and calcium/fat quantification on non-contrast chest CT images. This talk introduces the technology, benefits, and real-world applications of CT data from Taiwan's National Health Insurance Administration. Our research aims to enhance patient care by providing an effective tool for identifying and measuring heart disease, ultimately leading to better treatment and outcomes.

## [02533] Reliable and Efficient Numerical Computation of Nonlocal Models

**Session Time & Room :** 2C (Aug.22, 13:20-15:00) @G709

**Type :** Proposal of Minisymposium

**Abstract :** Nonlocal models, which have proven effective in capturing long-range interactions in diverse applications, often involve integrals over a nonlocal horizon. Proper numerical discretization of these integrals is essential to ensure reliable and efficient simulations of the models. This requires addressing issues such as efficiently evaluating nonlocal integrals with domain-specific and computationally suitable meshes, as well as ensuring robustness as the size of the nonlocal horizon approaches zero. This minisymposium provides a platform for researchers to share their experiences and insights on designing reliable and efficient numerical schemes for nonlocal models.

**Organizer(s) :** Kuang Huang, Xiaobo Yin

**Classification :** 35R09, 65R20

**Minisymposium Program :**

02533 (1/1) : 2C @G709 [Chair: Kuang Huang]

## [03174] The Effect of Domain Truncation for Nonlocal Models and Asymptotically Compatible Schemes in Numerical Computation

**Format :** Talk at Waseda University

**Author(s) :** Xiaobo Yin (Central China Normal University)Qiang Du (Columbia University)Hehu Xie (Academy of Mathematics and Systems Science, Chinese Academy of Sciences)Jiwei Zhang (Wuhan University)

**Abstract :** Many nonlocal models have adopted a finite and radially symmetric nonlocal interaction neighborhoods. When solving them numerically, it is sometimes convenient to adopt polygonal approximations of such interaction neighborhoods. A crucial question is, to what extent such approximations affect the nonlocal operators and the corresponding nonlocal solutions. While recent works have analyzed this issue for nonlocal operators in the case of a fixed horizon parameter, the question remains open in the case of a small or vanishing horizon parameter, which happens often in many practical applications and has significant impact on the reliability and robustness of nonlocal modeling and simulations. In this report, we are interested in addressing this issue and establishing the convergence of new nonlocal solutions by polygonal approximations to the local limit of the original nonlocal solutions. Our finding reveals that the new nonlocal solution does not converge to the correct local limit when the number of sides of polygons is uniformly bounded. On the other hand, if the number of sides tends to infinity, the desired convergence can be shown. We also apply this finding to discuss of the asymptotically compatible property of the numerical schemes.

## [03775] Global well-posedness of one new class of initial-boundary value problem on incompressible Navier-Stokes equations and the related models

**Format :** Talk at Waseda University

**Author(s) :** Shu Wang (Beijing University of Technology)

**Abstract :** The global well-posedness of the initial-boundary value problem on incompressible Navier-Stokes equations and the related models in the domain with the boundary is studied. The global existence of a class of weak solution to the initial boundary value problem to two/three-dimensional incompressible Navier-Stokes equation with the pressure-velocity relation at the boundary is obtained, and the global existence and uniqueness of the smooth solution to the corresponding problem in two-dimensional case is also established. Some extends to the corresponding incompressible fluid models such as Boussinesq equation/MHD equations and FSI models etc. are given.

## [04201] High performance implementation of 3D FEM for nonlocal Poisson problem

**Format :** Online Talk on Zoom

**Author(s) :** JIWEI ZHANG (Wuhan University )

**Abstract :** Nonlocality brings many challenges to the implementation of finite element methods (FEM) for nonlocal problems, such as large number of queries and invoke operations on the meshes. Besides, the interactions are usually limited to Euclidean balls, so direct numerical integrals often introduce numerical errors. The issues of interactions between the ball and finite elements have to be carefully dealt with, such as using ball approximation strategies.

In this talk, an efficient representation and construction methods for approximate balls are presented based on combinatorial map, and an efficient parallel algorithm is also designed for assembly of nonlocal linear systems. Specifically, a new ball approximation method based on Monte Carlo integrals, i.e., the fullcaps method, is also proposed to compute numerical integrals over the intersection region of an element with the ball.

## [03599] Asymptotical compatibility of a class of numerical schemes for a nonlocal traffic flow model

**Format :** Talk at Waseda University

**Author(s) :** Kuang Huang (Columbia University)Qiang Du (Columbia University)

**Abstract :** This talk presents a study of numerical schemes for a nonlocal conservation law modeling traffic flows with nonlocal inter-vehicle interactions. We demonstrate the asymptotical compatibility of a class of finite volume schemes with suitable discretizations of the nonlocal integral. The numerical solutions produced by the schemes converge to the weak solution of the nonlocal model with a fixed nonlocal horizon and to the weak entropy solution of the respective local model as the mesh size and nonlocal horizon parameter go to zero simultaneously. Our findings provide insight into the development of robust numerical schemes for nonlocal conservation laws.

## [02537] Structured Low-Rank Matrices and Their Applications

**Session Time & Room :**

02537 (1/2) : 2D (Aug.22, 15:30-17:10) @A601

02537 (2/2) : 2E (Aug.22, 17:40-19:20) @A601

**Type :** Proposal of Minisymposium

**Abstract :** Large dense matrices are ubiquitous in engineering and data science applications, e.g. preconditioners for iterative boundary integral solvers, frontal matrices in sparse multifrontal solvers, and computing the determinant of covariance matrices. Such dense matrices have a numerical low-rank structure, which can be exploited to reduce the complexity of matrix multiplication and factorization from cubic to (near-)linear. As mixed-precision and randomized linear algebra become commonplace, such approximations become increasingly important.

**Organizer(s) :** Rio Yokota, Hatem Ltaief

**Classification :** 65Rxx, 15Axx, 41Axx, 65Yxx, 65Nxx**Minisymposium Program :**

02537 (1/2) : 2D @A601 [Chair: Rio Yokota]

**[05519] Hierarchical Lowrank Arithmetic with Binary Compression****Author(s) :** Ronald Kriemann (Max Planck Institute for Math. i.t.S.)**Abstract :** With lowrank approximation the storage requirement for dense data is reduced to linear levels. However, the lowrank factors are often stored using double precision. Newer approaches exploit the different IEEE754 floating point formats in a mixed precision approach. Since these formats show a significant storage (and accuracy) gap, we look beyond the standard formats and use an adaptive precision scheme to further increase the storage efficiency and investigate its effects on the arithmetic of H-matrices.**[05545] Parallel Factorization of Hierarchical Matrices****Author(s) :** Wagih Halim Boukaram (Lawrence Berkeley National Lab)**Abstract :** Hierarchical matrices allow for memory efficient representation of the data sparse matrices that often appear in scientific applications. The open source H2Opus library provides distributed CPU and GPU implementations of several key operations using the H2-variant of hierarchical matrices, where nested row and column bases allow for asymptotically optimal memory storage requirements. In this talk, we discuss the details of a newly developed parallel hierarchical factorization algorithm using skeletonization.**[05552] Parallel Low-Rank Approximation of High-Dimensional Multivariate Normal Probabilities on Manycore Systems****Author(s) :** Xiran Zhang (KAUST)Sameh Abdulah (KAUST)Hatem Ltaief (KAUST)Ying Sun (KAUST)Marc Genton (KAUST)David Keyes (KAUST)**Abstract :** The multivariate normal (MVN) probabilities frequently appear in statistics to support applications requiring, for example, the computation of skewed probability density functions or Bayesian spatial probit problems. In the literature, the separation-of-variable (SOV) technique is commonly used to compute the MVN probability by converting the integration region to the unit hypercube, allowing a faster convergence rate. However, the SOV techniques require the computation of the Cholesky factorization of an  $n \times n$  matrix with  $O(n^3)$  computation and  $O(n^2)$  space complexity. The computing of the Cholesky factorization operation in higher dimensions is prohibitive in dense structures. Thus, several studies have proposed to include an approximation technique that can help perform the Cholesky factorization faster while preserving the required accuracy. Another direction is to rely on high-performance computing techniques to allow intensive computing on modern parallel systems. In this work, we aim to couple the computing power and the hierarchical approximation to allow faster computation of the MVN probability of high-dimensional problems. We rely on state-of-the-art parallel hierarchical linear algebra algorithms and runtime systems to provide high performance and scalability in computing the MVN probability. We also include a block reordering technique to allow a faster convergence rate than the dense algorithm. Moreover, we assess the performance and the accuracy of the provided method using simulations and real air pollution data.**[05590] A geometry oblivious H-matrix approximation scheme for rectangular matrices****Author(s) :** George Biros (The University of Texas at Austin)**Abstract :** We propose a novel method for compressing dense matrices. Our method is based on a hierarchical-matrix (H-matrix) approximation. H-matrix approximations have been popular in science and engineering applications. They combine the notion of singular value decomposition (SVD) with appropriate block permutations and recursion. H-matrices are applicable to problems in which the matrix entries correspond to pairwise interactions between sets of points, as for example in kernel matrices. Here we generalize this approximation to arbitrary dense matrices. Our method comprises of a randomized low-rank approximation of permuted blocks along with approximate leverage scores computations that are used to find such

permutations. We introduce theoretical analysis, complexity analysis, and experimental results on kernel matrices.

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02537 (2/2) : 2E @A601 [Chair: Hatem Ltaief]

## [05551] Dynamic Rupture Simulation Using FDP Method Accelerated by Lattice H-matrices

**Author(s)** : Takumi Miyajima (The University of Tokyo) Akihiro Ida ( Japan Agency for Marine-Earth Science and Technology ) Ryosuke Ando (The University of Tokyo)

**Abstract** : Dynamic rupture simulation with the spatiotemporal boundary integral equation method requires  $N \times N$  dense matrices in a naive method. In order to reduce the memory consumption and computational cost, we propose a new approximation method called “FDP=LH matrices method” by incorporating travel time approximation into H matrices.

In this minisymposium, we will talk about the algorithm and simulation results.

## [02541] Biochemical reaction network reduction methods & multiple timescale dynamics

**Session Time & Room :**

02541 (1/2) : 2C (Aug.22, 13:20-15:00) @G402

02541 (2/2) : 2D (Aug.22, 15:30-17:10) @G402

**Type** : Proposal of Minisymposium

**Abstract** : The last couple of years has seen a flurry of research output on the topic of model reduction based on reactions evolving on disparate timescales. This minisymposium will provide the opportunity to present & discuss the state-of-the-art in this field from multiple angles spanning mathematical theory to synthetic biology and other biochemical applications, and its challenges.

**Organizer(s)** : Martin Wechselberger, Jae Kyoung Kim,

**Classification** : 34Exx, 37Cxx, 92Cxx, 14Txx

**Minisymposium Program :**

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02541 (1/2) : 2C @G402 [Chair: Martin Wechselberger]

## [04793] The relationship between deterministic and stochastic quasi-steady-state

**Format** : Talk at Waseda University

**Author(s)** : Jae Kyoung Kim (KAIST)

**Abstract** : The quasi steady-state approximation (QSSA) is frequently used to reduce deterministic models of biochemical networks. The resulting equations provide a simplified description of the network in terms of non-elementary reaction functions (e.g. Hill functions). Such deterministic reductions are frequently a basis for heuristic stochastic models in which non-elementary reaction functions are used as propensities of Gillespie algorithm. Despite the popularity of this heuristic stochastic simulations, it remains unclear when such stochastic reductions are valid. In this talk, I will present conditions under which the stochastic models with the non-elementary propensity functions accurately approximate the full stochastic models. If the validity condition is satisfied, we can perform accurate and computationally inexpensive stochastic simulation without converting the non-elementary functions to the elementary functions (e.g. mass action kinetics).

## [04404] Noise attenuation and ultrasensitivity in biological oscillators utilizing the multiple transcriptional repression mechanism

**Format :** Talk at Waseda University

**Author(s) :** Eui Min Jeong (Institute for Basic Science (IBS))Jae Kyoung Kim (Institute for Basic Science (IBS))Yun Min Song (KAIST)

**Abstract :** In many biological systems, multiple repression mechanisms are used together to inhibit transcriptional activators in many systems. This raises the question of what advantages arise from utilizing multiple repression mechanisms. Here, by deriving Fano factors and equations describing the multiple repression mechanisms, we find that their combination can reduce noise in the transcription while generating an ultrasensitive transcription response and thus, strong oscillation. This rationalizes why multiple repression mechanisms are used in various biological oscillators.

## [04800] Reduction of Chemical Reaction Networks with Approximate Conservation Laws

**Format :** Talk at Waseda University

**Author(s) :** Ovidiu Radulescu (University of Montpellier)Aurelien Desoeuvres (University of Montpellier)Alexandre Iosif (Rey Juan Carlos University of Madrid)Christopher Lueders (University of Bonn)Hamid Rahkooy (University of Oxford)Matthias Seiss (University of Kassel)Thomas Sturm (CNRS )

**Abstract :** Singular perturbation methods are used to reduce multiple timescale chemical reaction networks, but their practical applicability is limited by the manual identification of the small parameters required by the theory. Recently, we have shown that tropical geometry provides ways to rescale CRNs and to identify the small parameters used by singular perturbation theories. Here we consider the case when the fast subsystem has first integrals, not covered by our previous results.

## [04454] A deep dive into the quasi-steady-state approximation to the Michaelis-Menten system

**Format :** Online Talk on Zoom

**Author(s) :** Justin Spaulding Eilertsen (American Mathematical Society)

**Abstract :** Although the quasi-steady state approximation (QSSA) is justifiable from singular perturbation theory, the results addressing its accuracy rely on heuristic timescale estimates. We take a different approach. By combining phase plane analysis with differential inequalities, we obtain rigorous bounds on the accuracy of the QSSA. Moreover, under the assumption the QSSA is valid at the onset of the reaction, we obtain an error estimate that is order one in the Segel-Slemrod parameter.

02541 (2/2) : 2D @G402 [Chair: Jae Kyoung Kim]

## [04203] Multiple timescales in reaction networks and the parametrisation method

**Format :** Talk at Waseda University

**Author(s) :** Martin Wechselberger (University of Sydney)Ian Lizarraga (University of Sydney)Bob Rink (Vrije Universiteit Amsterdam)

**Abstract :** Many biochemical reaction network problems display distinct temporal features, which can be attributed to processes taking place on multiple timescales. In mathematical terms, such multiple timescale models are in fact singular perturbation problems. We present a parametrisation method for computing slow manifolds and their fast fibre bundles in such singular perturbation problems. In particular, we highlight the emergence of hidden timescales and show how our method can uncover these surprising multiple timescale structures.

# [02545] Challenges and Recent Advances in Phylogenetics

## **Session Time & Room :**

02545 (1/4) : 1D (Aug.21, 15:30-17:10) @A508

02545 (2/4) : 1E (Aug.21, 17:40-19:20) @A508

02545 (3/4) : 2D (Aug.22, 15:30-17:10) @A508

02545 (4/4) : 2E (Aug.22, 17:40-19:20) @A508

## **Type :** Proposal of Minisymposium

**Abstract :** Phylogenetic trees and networks are used to elucidate the evolutionary history of genes or species. Data proliferation due to recent technological advancements has led to the pursuit of more efficient algorithms and novel approaches. Advances in the area can lead to breakthroughs in various disciplines of biology and life sciences, including genetics, cell biology, zoology, botany, microbiology, epidemiology, drug discovery, and biodiversity conservation, to name a few. This mini-symposium will cover recent topics related to phylogenetic research, from both theoretical and practical viewpoints, with results from algebra, algorithms, bioinformatics, combinatorics, computational complexity, geometry, statistics, and software development.

**Organizer(s) :** Momoko Hayamizu, Yuki Murakami, Koyo Hayashi, Hiroshi Hirai

**Classification :** 92D15, 92B10, 62G07, 05C85, 05A15

## **Minisymposium Program :**

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02545 (1/4) : 1D @A508 [Chair: Yukihiro Murakami]

## [04132] Navigating the Frontiers of Phylogenetic Research: Challenges and Applications

### **Format :** Talk at Waseda University

**Author(s) :** Momoko Hayamizu (Department of Applied Mathematics, Waseda University)

**Abstract :** This talk serves as an introduction to our mini-symposium on phylogenetic research. It emphasizes key challenges and applications in this rapidly evolving field from both theoretical and biological perspectives. After providing a brief overview of the symposium topics and presentations, I will discuss some of the recent results and open problems related to phylogenetic trees and networks, with a focus on combinatorial and algorithmic approaches.

## [05050] Advances and challenges in statistical inference of phylogenetic networks

### **Format :** Talk at Waseda University

**Author(s) :** Luay Nakhleh (Rice University)

**Abstract :** Evolutionary analyses of various groups of eukaryotic species have revealed evidence for reticulation. Reticulate evolutionary histories are best represented as phylogenetic networks. I will describe the multispecies network coalescent (MSNC) model, which allows for modeling vertical and horizontal evolutionary processes acting within and across species boundaries. I will then discuss progress we have made on developing statistical inference methods under the MSNC as well as challenges facing the inference in practice.

## [03613] The Tree of Blobs of a Species Network: Identifiability

### **Format :** Online Talk on Zoom

**Author(s) :** Hector D Banos (California State University San Bernardino)Elizabeth S Allman (University of Alaska Fairbanks)John A Rhodes (University of Alaska Fairbanks)Jonathan D Mitchell (Univeristy of Tasmania)

**Abstract :** As genealogical analyses of DNA data have progressed, more evidence has appeared showing that hybridization is often an important factor in evolution. Hybridization has played a crucial role in the evolutionary history of plants, some groups of fish, and frogs, among other species. In such cases, networks are the objects used to represent the relationships between species. The network multispecies coalescent model is a standard probabilistic model describing the formation of gene trees in the presence of hybridization and incomplete lineage sorting. We present a step toward inferring a general species network by showing the identifiability of its tree of part\_2

blobs, in which all 'hybrid species relationships' are contracted to nodes, so only tree-like relationships between the taxa are shown.

## [03991] Identifiability of phylogenetic networks

**Format :** Talk at Waseda University

**Author(s) :** Leo van Iersel (TU Delft)

**Abstract :** Will we ever be able to reconstruct our own history and the history of other species? What can we reconstruct when we have enough data? And what cannot be reconstructed no matter how much data we collect? Evolutionary histories can be described using directed graphs called phylogenetic networks. Which phylogenetic networks can in principle be reconstructed from data of currently living species, like DNA data, under certain models of evolution? This is an important question to answer in order to be able to develop statistically-consistent methods. I will discuss algorithmic, graph theoretic and algebraic results that are important for answering this question.

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02545 (2/4) : 1E @A508 [Chair: Koyo Hayashi]

## [04778] Log-concave density estimation on tree space

**Format :** Talk at Waseda University

**Author(s) :** Yuki Takazawa (The University of Tokyo) Tomonari Sei (The University of Tokyo)

**Abstract :** A probability density is log-concave if its logarithm is concave. In recent decades, the maximum likelihood estimation method for log-concave densities has been developed in Euclidean spaces. In this talk, we introduce a generalization of this estimator to the space of phylogenetic trees. We provide a sufficient condition for the existence of the estimator, present the estimation algorithm, and discuss some challenges in the computation.

## [03260] Tropical Logistic Regression Model on Space of Phylogenetic Trees

**Format :** Talk at Waseda University

**Author(s) :** Ruriko Yoshida (Naval Postgraduate School) George Aliatimis (University of Lancaster) Burak Boyaci (University of Lancaster) James Grant (University of Lancaster)

**Abstract :** In recent years, tropical geometry has found applications in statistical learning over the space of phylogenetic trees. In this talk, we propose an analogue of the logistic regression model in the setting of tropical geometry. Our proposed method is to classify gene trees over the space of ultrametrics, a tropical linear space. The generalization errors of our model is discussed. Experiment results with simulated and empirical data show our model works well.

## [04319] From phylogenetics to semigroups, through set partitions

**Format :** Online Talk on Zoom

**Author(s) :** Andrew Francis (Western Sydney University)

**Abstract :** We show that the set of all phylogenetic trees and forests are in correspondence with the set of all partitions of finite sets, extending Diaconis and Holmes (1998). This correspondence can be further extended to phylogenetic networks through a class of covers of finite sets. Partitions of finite sets can be represented as diagrams in a partition monoid, leading to applications of semigroups in phylogenetics. Joint work with Peter Jarvis and with Mike Steel.

## [04284] Learning from phylogenies to uncover evolutionary dynamics

**Format :** Talk at Waseda University

**Author(s) :** Olivier GASCUEL (CNRS - Institut de Systématique, Evolution, Biodiversité (ISYEB))

**Abstract :** I will describe the work done in my group to estimate the parameters of models used in phylodynamics and macroevolution studies. In particular, we use neural networks combined with simulations to learn to predict the parameters of these models. This involves both adequate representations of phylogenies and the use of appropriate neural architectures. The results compare favourably with the state of the art, with extremely fast methods for analyzing very large trees.

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02545 (3/4) : 2D @A508 [Chair: Hiroshi Hirai]

## [05365] Minimum Number of Leaf-Covering Subtrees Covering Phylogenetic Networks

**Format :** Talk at Waseda University

**Author(s) :** Yuki Yoshida (The University of Tokyo)

**Abstract :** Several deviation measures of non-tree-based phylogenetic networks from tree-based have been defined and their characteristics have been studied. One of the measures is the minimum number of leaf-covering subtrees which cover the phylogenetic network. In this talk, I suggest the first polynomial-time and efficient algorithm to compute both the minimum number and the covering subtrees. This algorithm is based on flow algorithms on several networks transformed from the network used to compute another deviation measure.

## [04243] Proximity measures for phylogenetic network classes

**Format :** Talk at Waseda University

**Author(s) :** Yukihiro Murakami (TU Delft)Leo van Iersel (TU Delft)Mark Jones (TU Delft)Esther Julien (TU Delft)

**Abstract :** Orchard networks represent the evolutionary history of species as a tree structure with horizontal arcs. In this talk, we will explore the extent to which a network departs from being orchard. We will examine this deviation through varying graph operations such as adding leaves and removing arcs, as well as via vertex labeling. To provide context, we will compare these findings to proximity measures for other classes of networks, including tree-based and tree-child networks.

## [03534] Data reduction rules to compute distances between phylogenetic trees

**Format :** Online Talk on Zoom

**Author(s) :** Simone Linz (University of Auckland)Steven Kelk (Maastricht University)Ruben Meuwese (Maastricht University )Simone Linz (University of Auckland)

**Abstract :** In evolutionary biology, phylogenetic trees are widely used to unravel the ancestral history of entities such as species or viruses. However, it is not uncommon to obtain different trees for the same data set. For example this can be due to methodological reasons. These tree incongruences motivate the use of distance measures in phylogenetics to quantify the dissimilarities between two phylogenetic trees. One popular distance between phylogenetic trees is called the tree bisection and reconnection (TBR) distance. Although this distance is NP-hard to compute, it is also fixed-parameter tractable. In this talk, we describe a series of results on the size of the TBR kernel, i.e. the size of two phylogenetic trees after pre-processing.

## [03576] Parsimony and the rank of phylogenetic flattenings

**Format :** Online Talk on Zoom

**Author(s) :** David Bryant (University of Otago)

**Abstract :** The standard models of sequence evolution on a phylogeny determine probabilities for every character or site pattern. A flattening is an arrangement of these probabilities into a matrix, with rows corresponding to all possible site patterns for one set of taxa and columns corresponding to all site patterns for another. Flattenings have been used to prove difficult results in phylogenetic mathematics and form the basis of several methods of phylogenetic inference. We provide an exact formula for the rank of these matrices based on parsimony scores.

02545 (4/4) : 2E @A508 [Chair: Momoko Hayamizu]

## [04303] Phylogenetic X-cactuses

**Format :** Talk at Waseda University

**Author(s) :** Taoyang Wu (University of East Anglia)

**Abstract :** In this talk we discuss X-cactus, a type of phylogenetic network which is essentially a cactus graph in which some vertices are labelled by elements from a set X of species. In this talk, we present a way to encode X-cactuses in terms of certain collections of X-partitions, and discuss a partial order on the set of X-cactuses, including an analysis of some properties of its least upper and greatest lower bounds.

## [05034] On the Sackin index of galled trees

**Format :** Talk at Waseda University

**Author(s) :** Michael Fuchs (National Chengchi University)Bernhard Gittenberger (TU Wien)

**Abstract :** We will compute the Sackin index of some classes of phylogenetic networks that belong to so-called galled trees. In particular, we consider level-1 networks as well as the closely related one-component galled trees. The Sackin index is the sum of the vertex heights.

The method we approach the problem is specifying the networks in terms of combinatorial structures and performing a singularity analysis on the resulting generating functions.

## [04250] Distribution of patterns in ranked tree-child networks

**Format :** Talk at Waseda University

**Author(s) :** Michael Fuchs (National Chengchi University)Hexuan Liu (National Sun Yat-sen University )Tsan-Cheng Yu (National Chengchi University)

**Abstract :** In this talk, I will first review tree-child networks and ranked tree-child networks (RTCN), and then explain our results on the distributional behavior of certain patterns in random RTCNs. These results extend the limit law for cherries and give rise to a conjecture for general patterns. This is the first such study for a class of phylogenetic networks.

## [04323] Counting phylogenetic networks with the component graph method

**Format :** Talk at Waseda University

**Author(s) :** Michael Fuchs (National Chengchi University)

**Abstract :** The component graph method was proposed by Louxin Zhang in order to solve algorithmic problems for tree-child networks, galled networks, reticulation-visible networks and extensions. Moreover, the method was also used to obtain exact counting results of the number of networks with n leaves and k reticulations. In this talk, we will explain how we used the method to prove asymptotic counting results for tree-child networks with a fixed number of reticulation nodes and galled networks.

# [02557] Collaboration of machine learning and physics-based simulation on earthquake disasters

**Session Time & Room :**

02557 (1/2) : 1C (Aug.21, 13:20-15:00) @D408

02557 (2/2) : 1D (Aug.21, 15:30-17:10) @D408

**Type :** Proposal of Minisymposium

**Abstract :** In Japan, strong-ground-motion data have been accumulated over a quarter of a century by a nationwide observation network. Large-scale physics-based simulations using HPC have enabled evaluations that consider the uncertainties of natural phenomena. Studies have begun to make up for the observation data related to large-scale disasters, which are currently lacking, using these simulation data. Furthermore, as studies toward hazard and risk assessment, surrogate modeling and damage assessment modeling by machine learning using observation and simulation data are being performed. In this mini-symposium, we will introduce the collaborative research of machine learning and physics-based simulation mainly on earthquake disasters.

**Organizer(s) :** Takahiro Maeda, Takuzo Yamashita, Asako Iwaki, Ryuta Imai

**Classification :** 86A15, 68T07

**Minisymposium Program :**

02557 (1/2) : 1C @D408 [Chair: Takahiro Maeda]

## [04544] Physics-based long-period ground motion simulation for megaquakes

**Format :** Talk at Waseda University

**Author(s) :** Takahiro Maeda (National Research Institute for Earth Science and Disaster Resilience)

**Abstract :** There are limited seismic observation records directly linked to damage, such as ground motions caused by huge earthquakes and those near seismic faults. In order to evaluate such ground motions, physics-based seismic-ground-motion simulation using the three-dimensional subsurface structure and seismic-source models is carried out, which are used to clarify the causes of damage and predict future seismic motions. In this presentation, we will introduce ground-motion simulation methods and examples of their application to huge earthquakes.

## [03695] A smoothing scheme for seismic wave propagation simulation with SDWave

**Format :** Online Talk on Zoom

**Author(s) :** Ryuta Imai (Mizuho Research & Technologies, Ltd.)

**Abstract :** We propose a smoothing scheme SDWave for seismic wave propagation simulation. The SDWave is based on a diffusionized wave equation with the fourth-order spatial derivative term. We mathematically explain some properties of the equation and how the SDWave works for smoothing. Then we give two discretization methods, FDM and mixed FEM, of the SDWave and apply it to the wave equation. This numerical experiment reveals that the SDWave is effective for filtering short wavelength components.

## [04162] A quarter century of data from K-NET and KiK-net

**Format :** Online Talk on Zoom

**Author(s) :** Shin Aoi (National Research Institute for Earth Science and Disaster Resilience)Takashi Kunugi (National Research Institute for Earth Science and Disaster Resilience)Wataru Suzuki (National Research Institute for Earth Science and Disaster Resilience)Hiroyuki Fujiwara (National Research Institute for Earth Science and Disaster Resilience)

**Abstract :** Based on the lessons learned from the 1995 Kobe earthquake, the National Research Institute for Earth Science and Disaster Resilience (NIED) has constructed K-NET and Kik-net, nationwide strong-motion observation networks that homogeneously cover the entire country. The strong-motion database obtained from these world's largest strong-motion observation networks contains nearly one million archived records. In this presentation, these observation networks and databases will be introduced and the utilization of the data will be discussed.

## [05004] Construction of strong motion database for data-driven ground-motion prediction models

**Format :** Talk at Waseda University

**Author(s) :** Asako Iwaki (National Research Institute for Earth Science and Disaster Resilience)Nobuyuki Morikawa (National Research Institute for Earth Science and Disaster Resilience)Takahiro Maeda (National Research Institute for Earth Science and Disaster Resilience)Hiroyuki Fujiwara (National Research Institute for Earth Science and Disaster Resilience)

**Abstract :** We have been developing a strong-motion observation database as an infrastructural database utilized for seismic hazard assessment, from which data-driven regression models for ground-motion prediction (ground-motion models; GMMs) are to be constructed. The database is "biased" because there are insufficient number of records with large magnitudes and short distances. Consequently, GMMs are incapable of predicting such ground motion. To overcome this issue, we attempt to utilize simulated ground motion data to supplement the observation database.

02557 (2/2) : 1D @D408 [Chair: Takuzo Yamashita]

## [03553] Optimal Transport in Seismic Wave Analysis

**Format :** Talk at Waseda University

**Author(s) :** Tomohisa Okazaki (RIKEN)

**Abstract :** An appropriate measure of the similarity between waveforms is crucial for seismic data analysis and modeling. The use of the Wasserstein distance in optimal transport theory has received attention in seismology because it captures time difference of waveforms. This presentation introduces two research directions: (1)

converting acceleration envelopes from long to short periods for predicting ground motions caused by scenario earthquakes; (2) the sliced Wasserstein distance between seismograms to efficiently measure the similarity of oscillating seismic signals. These applications support the effectiveness of the Wasserstein distance as a similarity measure of seismic waveforms.

## [03984] Position-dependent inpainting for ground motion interpolation

**Format :** Online Talk on Zoom

**Author(s) :** Hirotaka Hachiya (Wakayama University)

**Abstract :** Acquiring continuous spatial data is essential to assess the damaged area just after the earthquake. To this purpose, we propose a framework of supervised spatial interpolation and apply highly advanced deep inpainting methods with the introduction of position-dependent partial convolution, where convolution kernel weights are adjusted depending on their position on an image based on the trainable position-feature map. We show the effectiveness of our proposed method, through experiments using ground-motion data.

## [04967] Linkage of physics simulation and machine learning towards seismic risk assessment

**Format :** Talk at Waseda University

**Author(s) :** Takuzo Yamashita (NIED)Jun Fujiwara (NIED)Asako Iwaki (NIED)Hiroyuki Fujiwara (NIED)

**Abstract :** The authors are developing a seismic risk assessment method with physical simulation and machine learning. Response surfaces of seismic demand are modeled by Gaussian process regression. Low-dimensional features of seismic motions with auto-encoder were used as input data. An active learning method using Bayesian optimization was developed to construct the model with a small number of samplings. As a result, proposed model using samples less than 1/10th of the total data successfully predicted correct values.

## [03740] Automated Building Damage Assessment using Multi-scale Siamese Deep Learning Network

**Format :** Talk at Waseda University

**Author(s) :** Bahareh Kalantar (RIKEN AIP)Naonori Ueda (RIKEN AIP)

**Abstract :** Timely information on building damage location is vital for emergency responders after natural disasters. Our proposed Multi-scale Siamese Building Damage Assessment model assesses damage by localizing buildings and classifying damage level into four categories. The model employs a multi-scale block to handle buildings of varying sizes. The results indicate the model's effectiveness, although it struggles with classifying minor and major damage.

# [02561] Mathematical Puzzles and Games in Theoretical Computer Science

**Session Time & Room :**

02561 (1/2) : 1D (Aug.21, 15:30-17:10) @G601

02561 (2/2) : 1E (Aug.21, 17:40-19:20) @G601

**Type :** Proposal of Minisymposium

**Abstract :** Research on puzzles and games from the viewpoint of theoretical computer science has continued without any break in the history of theoretical computer science. Sometimes the research on computational complexity classes has proceeded by understanding the tons of puzzles. The wide collection of complete problems for a specific computational complexity class shares a common property, which gives us a deep understanding of the class. In this mini-symposium, we will explore the latest topics, results, and trends related to puzzles and games from the viewpoints of mathematics and theoretical computer science.

**Organizer(s) :** Ryuhei Uehara

**Classification :** 03D15, 52C45, 68Q15

**Minisymposium Program :**

## [04517] Uniqueness in puzzles and puzzle solving

**Format :** Talk at Waseda University

**Author(s) :** David Eppstein (University of California, Irvine)

**Abstract :** Many classical pencil-and-paper puzzles are defined in a way that requires the puzzle to have a unique solution. We explore the theoretical and practical implications of this requirement on the difficulty of puzzle-solving and puzzle generation, and the uses of the assumption of uniqueness in puzzle inference rules for puzzles including Sudoku, Slither Link / Loopy, and Map.

## [04855] The Complexity of Games and Puzzles with Limited Width

**Format :** Talk at Waseda University

**Author(s) :** Tom van der Zanden (Maastricht University)

**Abstract :** When studying the complexity of games and puzzles, we usually consider generalized versions. For example, chess is played on an  $8 \times 8$  board but when analyzing the complexity, we consider a version played on an  $n \times n$  board. What if instead we consider the  $n \times k$  variant, where  $k$  is a small number? In this talk, we survey some results on the computational complexity of games and puzzles with small width.

## [04898] Mathematical Puzzles for Computer Scientists: Leisure or More?

**Format :** Talk at Waseda University

**Author(s) :** Hirokazu Iwasawa (Waseda University)

**Abstract :** The speaker, a creator of mathematical puzzles including mechanical puzzles, introduces a selection of puzzles that are likely to appeal to computer scientists, chosen from those he has devised in the past. While these puzzles can be enjoyed as leisure, some of them may potentially become subjects of research.

## [05028] One Cycle to Rule Them All

**Format :** Talk at Waseda University

**Author(s) :** Giovanni Viglietta (University of Aizu)

**Abstract :** One of the consequences of the classification of the finite simple groups is that, if  $G$  is a primitive permutation group of degree  $n$  containing a cycle of length  $n - 3$  or less, then  $G$  is either the symmetric group  $S_n$  or the alternating group  $A_n$ . We will discuss some applications of this result to the theory of token permutation puzzles, as well as some open problems and directions for further research.

02561 (2/2) : 1E @G601 [Chair: Ryuhei Uehara]

## [05095] Generalized Jankens

**Format :** Talk at Waseda University

**Author(s) :** Hiro Ito (University of Electro-Communications)

**Abstract :** Janken or rock-paper-scissors, which is a very simple game and it is usually used as a coin-toss in Japan, originated in China, and many variants are seen throughout the world. A variant of janken can be represented by an asymmetric digraph, where a vertex corresponds a sign and an arc  $(x,y)$  means sign  $x$  defeats sign  $y$ . However, not all asymmetric digraphs define useful janken variants, i.e., some janken variants may include a useless sign, which is strictly inferior than another sign in any case. We call a janken variant efficient if it contains no such a useless sign. We also introduced a measure of amusement of janken variants. We show the results of our mathematical research on janken variants.

## [05219] Tilings and unfoldings

**Format :** Talk at Waseda University

**Author(s) :** Stefan Langerman (Université libre de Bruxelles)

**Abstract :** A tiling is a covering of the plane with copies of a geometric shape (tiles) without gaps or overlaps. A tiler is a shape that tiles the plane.

An unfolding is obtained by cutting along the surface of a polyhedron through all its vertices, and opening all the dihedral angles between adjacent faces to obtain a single flat non-overlapping geometric shape.

In this talk, I will explore connections between these fascinating concepts, highlight some recent results and mention several still unsolved algorithmic problems,

## [05433] A Hardness Framework for Games and Puzzles: Motion Planning through Gadgets

**Format :** Talk at Waseda University

**Author(s) :** Erik D. Demaine (Massachusetts Institute of Technology)

**Abstract :** Many games and puzzles, especially video games, involve one or more characters moving through a changeable environment, like Mario in Super Mario Bros. We describe a powerful framework for proving hardness of such games by characterizing which "gadgets" it suffices to build in the game. A gadget is a local piece of environment with limited traversals, some of which change local state, which in turn change available traversals, similar to a finite automaton. We prove that very simple gadgets suffice to prove NP-hardness, PSPACE-hardness, or EXPTIME-hardness. This framework enables many hardness proofs, old and new, to be distilled down to a single diagram of a single gadget, resulting in new or simplified hardness proofs for games such as Super Mario Bros., Mario Kart, Pokémon, Lemmings, Rush Hour, and Chess. It also opens up a rich study of gadgets themselves, including which gadgets can "simulate" which others, where a "simulation" is a graph representing a reduction algorithm.

## [05443] Map Folding

**Format :** Talk at Waseda University

**Author(s) :** Yushi Uno (Osaka Metropolitan University)

**Abstract :** Origami (paper folding) is not only a traditional Japanese entertainment, but also an interesting research topic in both engineering and computer science. One of the special cases of paper folding is map folding, and it has interesting open problems. In this talk, we will introduce the map folding problem and show their latest research results.

# [02562] Recent development in data-driven modeling, data assimilation, and applications: meteorology, oceanography ionosphere, hydrology, environment

**Session Time & Room :**

02562 (1/2) : 2C (Aug.22, 13:20-15:00) @G703

02562 (2/2) : 2D (Aug.22, 15:30-17:10) @G703

**Type :** Proposal of Minisymposium

**Abstract :** Multi-physics problems typically have essential dynamics. Numerical models are often hindered by difficulties in fully capturing the relevant physics. Nowadays, more attention has been given to data science approaches. A hybrid AI and multiscale physical modeling approach could be the optimal way to provide a dynamic understanding of the governing equations. Data-driven modeling results may find some patterns which are not expected from physical modeling. This session aims at exploring the challenges of physical and data-driven modeling for real-time prediction and applications to geosciences, addressing uncertainty quantification, data assimilation, high-performance computing, machine learning, numerical methods, and reduced order modeling.

**Organizer(s) :** Haroldo Fraga de Campos Velho, Fangxin Fang

**Classification :** 35Q30, 68W10, 65M22

**Minisymposium Program :**

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02562 (1/2) : 2C @G703 [Chair: Haroldo F. de Campos Velho]

## [04677] Adaptive mesh atmospheric model development

**Format :** Talk at Waseda University

**Author(s) :** Jinxi Li (Institute of Atmospheric Physics, Chinese Academy of Sciences)Fangxin Fang (Imperial College London)Pu Gan (Chengdu University of Information Technology)Christopher Pain (Imperial College London)Xiaofei Wu (Chengdu University of Information Technology)Zifa Wang (Institute of Atmospheric Physics, Chinese Academy of Sciences)Jie Zheng (Institute of Urban Environment, Chinese Academy of Sciences)Jiang Zhu (Institute of Atmospheric Physics, Chinese Academy of Sciences)

**Abstract :** This study presents the development of a three-dimensional unstructured adaptive finite-element model (Fluidity-Atmosphere) for atmospheric research. To improve the computational efficiency, a LSTM-based three-dimensional unstructured mesh generator is proposed to predict the evolution of the adaptive mesh. To evaluate the performance of adaptive meshes and physical parameterisations in Fluidity-Atmosphere, a series of idealized test cases have been setup and the unstructured tetrahedral meshes are adapted automatically with the specified fields in time and space.

## [05293] A fast, high resolution pluvial flood model for risk assessment and real-time flood prediction

**Format :** Talk at Waseda University

**Author(s) :** Steven Cocke (Florida State University)Dong-Wook Shin (Florida State University)

**Abstract :** A high resolution, computationally efficient pluvial flood model has been developed to provide flash flood inundation estimates due to heavy precipitation events. The need for a computationally fast model is critical for estimating flood risk, where a large number of flood scenarios are needed to obtain a reliable probability distribution of flood depths and extents, as well as for real-time prediction where sufficient advance warning must be given to the public.

## [04758] Data driven modelling and EnKF for spatial-temporal forecasting: Ozone and PM forecasting in China

**Format :** Talk at Waseda University

**Author(s) :** Fangxin Fang (Imperial College London)Meiling Cheng (Imperial College London)Shengjuan Cai (Imperial College London)Christopher Pain (Imperial College London)Yanghua Wang (Imperial College London)Michael I Navon (Florida State University)Jiang Zhu (Institute of Atmospheric Physics, Chinese Academy of Sciences)Jie Zhu (Institute of Urban Environment)Jinxi Li (Institute of Atmospheric Physics, Chinese Academy of Sciences)Xiaofei Wu (Chengdu University of Information Technology)

**Abstract :** Spatiotemporal forecasting involves generating temporal forecasts for system state variables across spatial regions. Data-driven methods, such as Convolutional Long Short-Term Memory (ConvLSTM) and deep convolutional generative adversarial network (DCGAN), are effective in capturing both spatial and temporal correlations. To further improve the predictive accuracy, the data assimilation EnKF is introduced to data driven modelling. Here, the performance of the data driven models has been demonstrated in hourly and daily spatiotemporal pollutant forecasting in China. The results have been compared to monitoring measurements and physical modelling results.

## [05285] Machine learning for data assimilation and predictability to the atmospheric models

**Format :** Talk at Waseda University

**Author(s) :** Haroldo Fraga de Campos Velho (INPE: National Institute for Space Research)Rosangela Cintra (INPE: National Institute for Space Research)Steven Cocke (FSU: Florida State University)Vinicius Albuquerque Almeida (UFRJ: Federal University of Rio de Janeiro)Juliana Aparecida Anochi (INPE: National Institute for Space Research)Vinicius Monego (INPE: National Institute for Space Research)

**Abstract :** Data assimilation is one of the most important challenges for the computational effort of the operational centers for weather and climate predictions. In this talk, the use of machine learning approaches will be shown for numerical weather models. Techniques for data assimilation for global and regional models are addressed by artificial neural networks. The analysis computed by self-configuring a supervised neural network for the COAPS-FSU global model is designed to emulate the Local Ensemble Transform Kalman filter. A deep learning neural network is applied to the WRF-NCAR regional model as a new method for data assimilation, where the 3D-Var scheme is employed as a reference to the machine learning approach. Our numerical experiments show a significant reduction in the CPU-time to calculate the analysis maintaining the precision of the forecasting for both models. Finally, another important issue is to evaluate how good is the prediction, in other words, how we can calculate the forecasting confidence interval. The standard procedure to compute the confidence interval is to apply

the ensemble prediction. A novelty approach to estimate the prediction uncertainty quantification is addressed by using machine learning algorithms: neural networks, and decision tree formulations.

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02562 (2/2) : 2D @G703 [Chair: Prof. Fangxin Fang]

### [05103] Prediction of Swirling Fluid Flow Pattern in a River

**Format :** Talk at Waseda University

**Author(s) :** Haradhan Maity (Rishi Bankim Chandra Evening College)

**Abstract :** Swirling of water in a river occurs when rocks, holes, obstacles, or sudden changes in the river channel obstruct the flow of the water. The swirl is characterized by turbulent parameters (velocities and Reynolds stresses) and corresponding factors associated with turbulence. The main objective of this study is to obtain the governing equations for swirling flow and to predict the flow pattern. The proposed theoretical models show very good agreement with experimental data.

## [02567] Data-driven Computational Mechanics for Structures, Structural Dynamics, and Materials

**Session Time & Room :**

02567 (1/3) : 4E (Aug.24, 17:40-19:20) @D102

02567 (2/3) : 5B (Aug.25, 10:40-12:20) @D102

02567 (3/3) : 5C (Aug.25, 13:20-15:00) @D102

**Type :** Proposal of Minisymposium

**Abstract :** Topics of this mini-symposium include, but not limited to, data-driven methods; incorporation of machine learning techniques; uncertainty quantification, and inverse problems in structures, structural dynamics and materials. Special emphasis is on the fields of structures, structural dynamics and materials with large-scale industry-relevant problems. Potential topics also include integrated modeling and design optimization, multiscale/multi-physics simulation based on the relevant data-driven process. The mini-symposium will bring together researchers working on both fundamental and applied aspects of data-driven computational mechanics to provide a forum for discussion, interaction, and assessment of techniques.

**Organizer(s) :** Haeseong Cho, Youngsoo Choi, SangJoon Shin

**Classification :** 74-10, 35Q74, 35Q68, 70-10, 68T07

**Minisymposium Program :**

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02567 (1/3) : 4E @D102

### [03299] Investigation on the hyper-reduction approach for the contact-impact simulation

**Author(s) :** SANGJOON SHIN (Seoul National University)Seung-Hoon Kang (Seoul National University)Minho Hwang (Seoul National University)Yongse Kim (Republic of Korea Air Force)Haeseong Cho (Jeonbuk National University)

**Abstract :** In the multi-body finite element analysis, the contact algorithm usually requires huge computational cost to capture the temporal/spatial discontinuity on the contact surface. This presentation will investigate the projection-based reduced-order model for the contact-impact simulation. Discrete empirical interpolation method (DEIM) will be employed among the hyper-reduction approaches for computation acceleration. Treatment on each nonlinear component, internal and contact force vectors, will be examined for the generation of DEIM basis and sparse sampling.

## [03428] Machine learning-based methods for the nonlinear structural analysis

**Author(s)** : Sangmin Lee (Seoul National University)SiHun Lee (Seoul National University)Haeseong Cho (Jeonbuk National University)SANGJOON SHIN (Seoul National University)

**Abstract** : Nonlinear structural analysis plays an important role in many fields of engineering, but it requires substantial computational resources to conduct repetitive high-fidelity simulation. In this study, a machine learning based non-intrusive model order reduction (MOR) is proposed for the parameterized structural analysis in which the geometric nonlinearities are involved. For this purpose, the proper orthogonal decomposition (POD) is carried out to gather the reduced bases from the full-order snapshot matrix. Then, the modified nouveau variational autoencoder (mNVAE) is conducted to interpolate such POD coefficients.

## [05003] Manifold-Augmented Deep learning-based Approach for Prediction of Airfoil Aerodynamic Performance at Low Reynolds Number

**Author(s)** : Seongwoo Cheon (Jeonbuk National University)Hyejin Kim (Jeonbuk National University)Seokhui Ryu (Gyeongsang National University)Haeseong Cho (Jeonbuk National University)Hakjin Lee (Gyeongsang National University)

**Abstract** : Computational fluid dynamics (CFD) analysis usually gives an accurate performance, better reliability, but it requires intensive computational time and cost. In this study, the deep learning-based MOR framework is proposed to predict the aerodynamic performance of airfoils. For this purpose, the proper orthogonal decomposition (POD), autoencoder (AE), and variational autoencoder (VAE) is carried out to gather the latent vectors from full-order snapshot matrix. Moreover, a novel generative model using projection-based manifold learning is proposed to overcome the lack of data due to the computational cost of CFD analysis and augment the training data.

02567 (2/3) : 5B @D102

## [03424] Model Order Reduction for Fluid-Structure Interaction Analysis via the Data-driven Machine Learning

**Author(s)** : SiHun Lee (Seoul National University)Sangmin Lee (Seoul National University)Haeseong Cho (Jeonbuk National University)SANGJOON SHIN (Seoul National University)

**Abstract** : Analysis on the multi-disciplinary analysis such as a fluid-structure interaction usually requires huge computational time due to nonlinearity and interpolation. In this research, a completely data-driven model order reduction method is considered that is capable of the parametric estimation regarding fluid-structure interaction analysis. The proposed method first constructs a snapshot matrix that contains various parametric result and then, singular value decomposition (SVD) is conducted. By SVD, proper orthogonal decomposition (POD) modes and coefficients will be gathered, which is interpolated by the machine learning technique.

## [05031] Data-driven Model Reduction Approach for Multiscale Homogenization of Microstructure

**Author(s)** : Hyejin Kim (Jeonbuk National University)Dahan Song (Jeonbuk National University)Seongwoo Cheon (Jeonbuk National University)Haeseong Cho (Jeonbuk National University)

**Abstract** : Given the heterogeneous nature of composite materials at the microscopic level, computational multiscale homogenization can be employed to obtain effective macroscopic material properties. However, it requires significant computational resources for recursive procedures. In this study, an efficient data-driven homogenization method is proposed. Herein, a clustering-based data-driven model reduction and autoencoder are utilized to alleviate high-dimensional data, followed by the application of a recurrent network model to predict the stress field of microstructure from loading conditions.

## [05220] An efficient neural network approximation of entropy solutions

**Author(s)** : Donsub Rim (Washington University in St. Louis)Gerrit Welper (University of Central Florida)Randall J LeVeque (University of Washington)

**Abstract** : We show that a family of neural networks with fixed number of layers and degrees of freedom, can approximate any entropy solution to scalar conservation laws and furthermore, the embedded dynamics in the free parameters is linear regardless of the complexity of the solution.

02567 (3/3) : 5C @D102

## [04471] Hypernetwork-based low-rank neural ordinary differential equations for solving parameterized partial differential equations

**Author(s)** : Kookjin Lee (Arizona State University)Youngsoo Choi (Lawrence Livermore National Laboratory)Guangting Yu (Arizona State University)

**Abstract** : In this work, we propose a hypernetwork-based reduced order modeling approach for solving parameterized partial differential equations. The hypernetwork is trained to produce model parameters of latent dynamics models, which governs the evolution of reduced states in a low-dimensional manifold. We parameterize the latent dynamics as neural ordinary differential equations (NODEs). To improve the hypernetwork's inference capability, we develop a variant of NODEs, low-rank NODEs, where the model parameters are approximated in low-rank.

## [05436] High-dimensional regression using partition of unity networks (POU-Net)

**Author(s)** : Eric Felix Darve (Stanford University)Tiffany Fan (Stanford University)Nathaniel Trask (Sandia National Laboratories)Marta D'Elia (Stanford University)

**Abstract** : High-dimensional regression problems present challenges in scientific and engineering applications. Conventional approaches like polynomial interpolation become computationally expensive as the dimensionality increases exponentially. Sparse grids and radial basis function regression have been developed as alternatives, but they suffer from high computational costs, low accuracy, and instability in some cases. Deep Neural Networks (DNNs) have proven to be a reliable regression method for high-dimensional problems. However, designing an optimal DNN structure, weight initialization, and achieving high accuracy with the optimizer pose difficulties, making error control challenging in engineering and scientific applications. Additionally, reproducibility is often problematic. To address these issues, we introduce POU-Net and its variants. POU-Net takes advantage of DNNs' dimensionality reduction and regression capabilities. Additionally, it utilizes the reliability, accuracy, and computational efficiency of polynomial interpolation within the reduced dimension. Our approach enables robust and accurate regression across a wide range of input dimensions. We evaluate the proposed method using various benchmarks and applications, comparing its performance to state-of-the-art techniques.

## [05408] An augmented Lagrangian method to accelerate constrained optimization using hyperreduction

**Author(s)** : Tianshu Wen (University of Notre Dame)Matthew Zahr (University of Notre Dame)

**Abstract** : We present a numerical method to efficiently solve constrained optimization problems governed by large-scale nonlinear systems of equations using an augmented Lagrangian framework. A globally convergent, hyperreduced trust-region framework is embedded in the proposed framework to accelerate the optimization process in each major iteration. The trust-region framework constructs a hyperreduction model via empirical quadrature procedure on-the-fly, which completely avoids an offline training phase.

## [02569] Quantification of Business Uncertainties through Industrial Mathematics

**Session Time & Room :**

02569 (1/2) : 3C (Aug.23, 13:20-15:00) @D101

02569 (2/2) : 3D (Aug.23, 15:30-17:10) @D101

**Type** : Proposal of Industrial Minisymposium

**Abstract** : We are living in exceptional times, as trade conflicts, climate change and crises-related-pandemic are creating uncertainties that may influence the current business environment. Businesses face risks that are difficult to be measured. However, collaborative efforts among academia, industries, government and civil society through industrial mathematics will facilitate IN creating new sustainable ways of doing business in an unstable

part\_2

environment. This APCMfl minisymposium will discuss the handling and managing business uncertainties. Firstly, identification of challenges introduced by the uncertainties at operational and decision making, and secondly, the deliberation on the techniques in quantifying uncertainties and tackling the challenges.

**Organizer(s)** : Arifah Bahar, Zainal Abdul Aziz, Osamu Seiki, Kenji Kajiwara

**Classification** : 70L05, 70L10, 70L99, 81-08

**Minisymposium Program :**

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02569 (1/2) : 3C @D101 [Chair: OSAMU SAEKI]

## [03389] Mathematics behind performance estimation of multiscale structures

**Format** : Talk at Waseda University

**Author(s)** : Yichao Zhu (Dalian University of Technology)

**Abstract** : In business involving commercial products carrying multiscale structures, utilisation of uncertainty quantification tools that are both reliable and efficient is still needed. In this talk, appropriate use of mathematical techniques of asymptotic analysis is proposed to resolve the issue. As an example, uncertain behaviours of fibre-reinforced composite laminates are considered. Through asymptotic analysis, it is shown that the building blocks of such thin plate configurations are two-dimensional slices, and analytical solutions are even available in the situation in consideration. Correlations between the confidence interval about the plate bending stiffness and manufactural uncertainties can then be established with relative ease.

## [04204] Handling Uncertainties in Decision Making

**Format** : Online Talk on Zoom

**Author(s)** : ZAITUL MARLIZAWATI ZAINUDDIN (UTM CENTRE FOR INDUSTRIAL AND APPLIED MATHEMATICS (UTM-CIAM))NORSHELA NOH (UNIVERSITI TUN HUSSEIN ONN MALAYSIA (UTHM))ARIFAH BAHR (UTM CENTRE FOR INDUSTRIAL AND APPLIED MATHEMATICS (UTM-CIAM))

**Abstract** : This study highlights the importance of incorporating uncertainty quantification of stochastic parameters in stochastic programming compared to expert judgement approach. It proposes a methodology for integrating stochasticity of input parameters into two-stage stochastic programming. The approach involves constructing a binomial scenario tree, which combines a binomial tree for each stochastic parameter and discretizes the continuous probability distribution of the underlying stochastic process. The scenario tree consists of all possible scenarios to explain future situations.

## [04896] Aggregation value regression and its application to household demand forecasting

**Format** : Talk at Waseda University

**Author(s)** : Kei Hirose (Kyushu University)Hiroki Masuda (University of Tokyo)Hidetoshi Matsui (Shiga University)

**Abstract** : In recent years, a number of sensor data have been collected, and some researchers are interested in the aggregation values, such as congestion levels and electricity demand. This study constructs a regression modeling specifically designed for aggregation value forecasting. The proposed modeling is applied to household demand forecasting.

## [04885] Ensemble based approaches for business uncertainty quantification

**Author(s)** : Heri Kuswanto (Institut Teknologi Sepuluh Nopember)

**Abstract** : Uncertainty quantification becomes a crucial work in business modelling. Ensemble approaches have been proposed as one of the ways to quantify the uncertainty and has been proven to be a powerful method to generate more accurate predictions. The method belongs to the class of model combination, where the uncertainty is quantified by combining the information from several models through different ways. This talk will give an overview of ensemble-based approaches with some examples of applications.

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02569 (2/2) : 3D @D101 [Chair: OSAMU SAEKI]

## [04526] Topological methods for detection of uncertainties in Artificial Intelligence

**Format :** Talk at Waseda University

**Author(s) :** Hiroaki Kurihara (Artificial Intelligence Laboratory, Fujitsu Research, Fujitsu)

**Abstract :** Recently, with the development of AI technology, AI has been increasingly used for decision-making in various domains where sophisticated knowledge is required. Although well-trained AI models are used in such situations, AI has a weakness in that its predictive ability is reduced for data that was not included during training. In this talk, we will introduce a method to verify the uncertainty of the output of AI by observing the topological information of trained models.

## [04919] Consecutive eigenvalues distribution of asymmetric quantum Rabi models

**Format :** Talk at Waseda University

**Author(s) :** MASATO WAKAYAMA (NTT Institute for Fundamental Mathematics)

**Abstract :** We focus spectral structure of the asymmetric quantum Rabi models (AQRM), which are widely studied as one of the most fundamental models of light-matter interaction. Particularly, we will discuss the symmetric structure of the consecutive (i.e., nearest) eigenvalues of the AQRM when we vary the flip term, which is the symmetric-breaking parameter of the Hamiltonian.

## [05125] Changing the Misconception of Subsea Cable Laying Norm

**Format :** Talk at Waseda University

**Author(s) :** Kamaudin Ismail (Ifactors Sdn Bhd)

**Abstract :** The world today is undeniably heavily reliant on technology. As a result of the continuous advancement in technology, the demand for data transmission services is at an all-time high.

Subsea cables are one of the major foundation of global connectivity. It is responsible for transmitting 99% of international data traffic systemwide.

However, despite being crucial factor in global connectivity, the process of laying subsea cables is still widely misunderstood.

This paper aims to address this misconception and to shed lights on the real process of subsea cable laying.

A conventional cable laying concept is by mobilizing a dedicated cable lay vessel. However, the main issue in this equation is that the vessel can only be used for cable lay process alone.

The above concept above gave an opportunity for Ifactors to venture into an unknown open concept. It is a new technique/process which is modular and easier to setup for a short distance cable lay.

## [04095] Handling Uncertainties for Wastewater Treatment in Oxidation Pond

**Format :** Online Talk on Zoom

**Author(s) :** Zainal Abdul Aziz (Universiti Teknologi Malaysia)Arifah Bahar (Universiti Teknologi Malaysia)Amir Syafiq Hamzah (Universiti Teknologi Malaysia)

**Abstract :** Oxidation pond techniques are effective for wastewater treatment process due to low operational cost. A stochastic model accommodates the correlation between the phototrophic bacteria mPHO and pollutant existing in oxidation pond. The model analyses and handles the uncertainties of this process, particularly the effect of mPHO on the degradation of pollutant. The model parameters estimation use simulated maximum likelihood based on the real data collected from an oxidation pond located in Taman Timor, Johor, Malaysia.

# [02570] Parameter Estimation, Targeted Observation, and Data Assimilation in Coupled Systems

## **Session Time & Room :**

02570 (1/3) : 5B (Aug.25, 10:40-12:20) @D407

02570 (2/3) : 5C (Aug.25, 13:20-15:00) @D407

02570 (3/3) : 5D (Aug.25, 15:30-17:10) @D407

## **Type :** Proposal of Minisymposium

**Abstract :** This minisymposium focuses on the coupled weather/climate prediction systems, whose components are atmosphere, land surface, chemistry, etc.; topics include but not limited to parameter estimation, data assimilation, targeted observation, sensitivity analysis, uncertainty quantification, and predictability in the coupled systems.

**Organizer(s) :** Sujeong Lim, Ji Won Yoon, Xiaohao Qin, Ting-Chi Wu, Shigenori Otsuka

**Classification :** 86-10, 86A10, 47N50, 47N60, 90C31

## **Minisymposium Program :**

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02570 (1/3) : 5B @D407 [Chair: Shigenori Otsuka, Ji Won Yoon]

## [04638] Improving Numerical Forecast Skill: Combinational Parameter Optimization and Coupled Data Assimilation

### **Format :** Talk at Waseda University

**Author(s) :** Seon Ki Park (Ewha Womans University)

**Abstract :** Numerical weather prediction (NWP) requires coupled modeling and data assimilation, and its forecast skill depends on uncertainties in physical parameterizations and initial conditions. This study illustrates that NWP skill can be improved through optimization of physical parameterizations and data assimilation; the former includes combinational optimization which seeks for the optimal set of parameterizations followed by optimal parameter estimation, whereas the latter develops the coupled data assimilation systems such as the WRF-Noah LSM and the WRF-Chem.

## [05388] Application of the CNOP-PEP method in hydrological ensemble prediction in China to reduce model parameter uncertainties

**Author(s) :** Guodong Sun (Institute of Atmospheric Physics, Chinese Academy of Sciences)Mu Mu (Fudan University)

**Abstract :** In this talk, a conditional nonlinear optimal parameter perturbation ensemble prediction (CNOP-PEP) method is proposed. The CNOP-PEP method is employed to carry out ensemble prediction of evapotranspiration (ET) over Tibetan Plateau (TP). The numerical results show that ensemble prediction experiments conducted with the CNOP-PEP method exhibit better prediction skills compared to the reference ET over the TP. The prediction skill by employing the CNOP-PEP method is more excellent than those of the traditional methods.

## [05401] The effect of Westerly Wind Burst on ENSO

**Author(s) :** Youmin Tang (University of Northern British Columbia)

**Abstract :** Westerly wind bursts (WWBs), as a semi-stochastic process, play a vital role in El Niño–Southern Oscillation (ENSO). However, current dynamical models have large challenges in the representation of WWBs. In this study, we introduced and developed several WWB parameterization schemes, including a novel scheme developed using the deep learning technique. The effect of these parameterization schemes on ENSO simulation and prediction was comprehensively evaluated and systematically compared using coupled models with varied complexity.

## [04422] Improving Model Uncertainty in Physical Parameterizations: Combinational Optimizations Using Genetic Algorithm in the Coupled Atmosphere-Chemistry Model

**Format :** Talk at Waseda University

**Author(s) :** Ji Won Yoon (Ewha Womans University)

**Abstract :** The Asian dust storm is one of the important air pollution problems in South Korea; thus, it is significant to improve the air quality forecasting skill using a numerical prediction system. In this study, we developed an optimization system by applying the micro-genetic algorithm ( $\mu$ GA) interfaced with the Weather Research and Forecasting model coupled with Chemistry (WRF-Chem) to enhance air quality forecasting skills in East Asia. We introduce the results of the combinational optimizations.

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02570 (2/3) : 5C @D407 [Chair: Xiaohao Qin]

## [03616] A novel approach of data assimilation: application to ENSO diversity predictions

**Author(s) :** Wansuo Duan (Institute of Atmospheric Physics, Chinese Academy of Sciences)

**Abstract :** The talk introduces an approach of data assimilation (DA) entitled nonlinear forcing singular vector (NFSV) to neutralize combined effect of initial and model errors. The approach is applied to an intermediate-complexity ENSO model and reproduces the conditions of the emergence of both EP- and CP-El Niño events, eventually distinguishing El Niño types at two-season lead time in predictions. The NFSV-DA is a useful DA approach for offsetting initial and model error effects for ENSO predictions.

## [04195] Exploring data-driven sparse sensor placement for determining rain gauge locations

**Author(s) :** Daiya Shiojiri (Chiba University)Eiryo Kawakami (Chiba University)Shunji Kotsuki (Chiba University)

**Abstract :** This study explores the data-driven sparse sensor placement (SSP) to determine rain gauge locations for efficiently estimating the spatiotemporal interpolation of precipitation. The SSP determines the rain gauge locations using dominant modes extracted from spatiotemporal precipitation data over a training period. Through evaluations using radar-analyzed precipitation, we found that the SSP-based rain gauges enable to provide more accurate precipitation fields compared to the current operational rain gauge network in Japan.

## [04176] The Conditional Nonlinear Optimal Perturbation method and it's application to the targeting observation for tropical cyclones

**Author(s) :** Xiaohao Qin (LASG, Institute of Atmospheric Physics, Chinese Academy of Science)Mu Mu (Fudan University)Feifan Zhou (LACS, Institute of Atmospheric Physics, Chinese Academy of Science)Boyu Chen (Chinese Meteorology Administration)Jie Feng (Fudan University)

**Abstract :** To augment the routine observational network for better forecasts of tropical cyclones (TCs), targeting observations (TOs) have developed rapidly during the past several decades over China. In consequence, TC forecasts have benefitted a lot from these field campaigns. In this talk, research work and field campaigns of TOs are briefly overviewed. After that, we introduce a method named the conditional nonlinear optimal perturbation (CNOP), which is utilized to identify those areas should be additionally observed with priority in TOs. Using some examples, we explain how to use the CNOP method in mathematics, its impacts on improving TC forecasts, and its latest application in real time operational forecasts.

## [04998] Towards targeted observations of meteorological state for improving PM2.5 forecasts

**Author(s) :** Lichao Yang (Institute of Atmospheric Physics, Chinese Academy of Sciences)Wansuo Duan (Institute of Atmospheric Physics, Chinese Academy of Sciences)

**Abstract :** An advanced approach of conditional non-linear optimal perturbation (CNOP) was introduced to identify the sensitive area for targeted observations of meteorological fields associated with PM2.5 concentration forecasts of a heavy haze event that occurred in the Beijing-Tianjin-Hebei (BTH) region, China. We show numerically and physically that preferentially deploying additional observations in the sensitive areas identified by the CNOP approach can greatly improve the forecasting skill of PM2.5 forecasts.

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02570 (3/3) : 5D @D407 [Chair: Ting-Chi Wu, Sujeong Lim]

### **[03679] A case study of a dust event using the RAMS-MLEF atmosphere-aerosol coupled data assimilation system**

**Author(s)** : Ting-Chi Wu (Central Weather Bureau/International Integrated Systems, Inc.)Milija Zupanski (Colorado State University/Cooperative Institute for Research in the Atmosphere)

**Abstract** : This study demonstrates the capability of an atmosphere-aerosol coupled data assimilation RAMS-MLEF (Regional Atmospheric Modeling System - Maximum Likelihood Ensemble Filter) using a dust event over the Arabian Peninsula, which is an area known to be severely under-sampled. One important lesson learned is that the location and timing of observations largely determines the improvements achieved by data assimilation. The lack of observations also makes it very challenging to perform a quantitative verification of results.

### **[04249] Impact of Soil Moisture Observation in the Coupled Atmosphere-Land Data Assimilation System**

**Format** : Talk at Waseda University

**Author(s)** : Sujeong Lim (Ewha Womans University)Seon Ki Park (Ewha Womans University)Milija Zupanski (Colorado State University/Cooperative Institute for Research in the Atmosphere)

**Abstract** : Soil moisture is important in a coupled atmosphere-land surface model because it propagates to atmospheric variables in the planetary boundary layer through the latent and sensible heat fluxes. In this study, we introduce the results of the assimilation of both atmospheric and soil moisture observations within a strongly coupled data assimilation system, taking into account the cross-covariance between the atmosphere and land.

### **[04599] Application and improvement of Land Data Assimilation System at CWB**

**Author(s)** : PO-HSUN LIN (CWB / International Integrated Systems, Inc. (IISI))

**Abstract** : Interactions between land and atmospheric components are critical for coupled model forecasting. Improved accuracy of soil initial conditions has been shown to enhance land-atmosphere interactions in coupled processes. The Central Weather Bureau of Taiwan has collaborated with the National Center for Atmospheric Research to optimize the use of the High-Resolution Land Data Assimilation System in order to improve the deterministic forecast over Taiwan. The results of this collaboration will be presented in this summary.

## **[02578] Interfaces and Mixing – Conservation Laws and Boundary Value Problems**

**Session Time & Room :**

02578 (1/4) : 1E (Aug.21, 17:40-19:20) @G704

02578 (2/4) : 2C (Aug.22, 13:20-15:00) @G704

02578 (3/4) : 2D (Aug.22, 15:30-17:10) @G704

02578 (4/4) : 2E (Aug.22, 17:40-19:20) @G704

**Type** : Proposal of Minisymposium

**Abstract** : Interfaces and interfacial mixing and their non-equilibrium dynamics control a broad range of processes in nature, technology, industry, from supernovae and fusion to alternative energy sources and purification of water. Mathematically, these problems are extremely challenging to study in theory and in simulations. Analytically, one needs to solve the conservation laws, augmented with singular boundary value problem and ill-posed initial value problem. Numerical modeling imposes high demands on the accuracy, precision and the scale of computations. The mini-symposium builds upon recent achievements in understanding the dynamics of interfaces and mixing, and reports solutions for long-time challenges in fundamentals and applications.

**Organizer(s)** : Snezhana Abarzhi, James Glimm, Alexander Nepomnyashchy, Yasuhide Fukumoto

**Classification** : 35Q35

**Minisymposium Program :**

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02578 (1/4) : 1E @G704

## [03293] Interaction between a particle and a liquid surface

**Author(s)** : Alexander Nepomnyashchy (Technion - Israel Institute of Technology)

**Abstract** : The interaction of a particle with a liquid interface takes place in many engineering processes. We consider the motion of a spherical particle rising in a viscous fluid towards the interface. The particle mobility can be significantly modified

by a surfactant adsorbed on the interface. Upon the particle attachment to the interface, the spatial inhomogeneity of

the wetting properties on the particle surface strongly enhance the duration of the system equilibration.

## [03383] Smooth Navier-Stokes Solutions

**Author(s)** : James Glimm (Stony Brook University)

**Abstract** : Smooth Navier-Stokes solutions require a non-physical choice of entropy minimization, achieved constructively as a mean value relative to turbulent fluctuations. Other solutions are not smooth. Drivers of the proof are a turbulence analogue of renormalized perturbation theory, adapted from Quantum Field theory, and shown to be Borel resummable convergent on a dense set of turbulent states, together with the Foias theory of Young measures.

## [03416] Determining control parameters for unsteady pulling of mass-spectrometry emitters

**Author(s)** : Yvonne Stokes (The University of Adelaide)Gagani Pathumika Ranathunga (Oktal Sydac)Michael Chen (The University of Adelaide)

**Abstract** : Asymptotic modelling is used to examine the heating and pulling of an axisymmetric glass tube with an internal overpressure to form a taper with near-uniform bore and small wall thickness at the tip, as desired for mass-spectrometry emitters. There is no unique choice of pulling force and pressure to achieve the desired geometry, which is sensitive to the parameters. Phase plane plots are used to understand the dependence of the geometry on the control parameters.

## [03716] Front Tracking Simulations of reshocked Richtmyer-Meshkov Instability

**Author(s)** : Tulin Kaman (University of Arkansas)Ryan Holley (University of Arkansas)

**Abstract** : In this talk, we present an increasingly accurate and robust front tracking method for the numerical simulations of re-shocked Richtmyer-Meshkov Instability (RMI) of an air/SF<sub>6</sub> interface. The front-tracking with the weighted essentially non-oscillatory (WENO) schemes are compared with Collins and Jacob (2002) shock tube experiments. We study the effects of high-resolution high-order WENO simulations on the fine detail complex vortex roll-up structures and perform verification and validation studies to achieve good agreement between simulations and experiments.

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02578 (2/4) : 2C @G704

## [03735] Can environmental and intrinsic mechanisms of quantum mixing be distinguished experimentally?

**Author(s)** : Alexander Y Klimentko (The university of Queensland)Alexander Y. Klimentko (The university of Queensland)

**Abstract** : This presentation considers the possibility of quantum experiments that can, at least in principle, allow us to distinguish intrinsic and environmental mechanisms of decoherence. This experiment can be interpreted as a quantum-mechanical version of non-equilibrium mixing between two volumes separated by a thin interface. Decoherence is understood here as a general process that does not involve any significant exchanges of energy and is governed by a particular class of Kraus operators. This presentation considers different regimes of quantum tunnelling in the presence of different types of decoherence and shows that, at least under some conditions,

part\_2

intrinsic and environmental types of decoherence affect the tunnelling rates differently and, therefore, can be distinguished experimentally.

## [03969] Exact solutions to nonlinear difference equations associated with Hénon maps

**Author(s)** : Chihiro Matsuoka (Osaka Metropolitan University)Koichi Hiraide (Osaka Metropolitan University)

**Abstract** : We present exact solutions in non-integrable systems, taking the Hénon map as an example. The obtained solutions describe the stable and unstable manifolds at saddle fixed points and make it possible to calculate such invariant manifolds with complex structures. Using the obtained functions, we visualize the hyperbolic system encircling KAM tori and the Hénon attractor, in which chaotic orbits are captured accurately.

## [03994] Nonlinear interaction of two nonuniform vortex interfaces and large vorticity amplification

**Author(s)** : Katsunobu Nishihara (Osaka University)Chihiro Matsuoka (Osaka Metropolitan University)

**Abstract** : Vortex dynamics is an important research subject for geophysics, engineering and plasma physics. The nonlinear interaction of two nonuniform vortex interfaces with density stratification is investigated using the vortex sheet model. When a strong vortex sheet approaches a weaker vortex sheet with opposite-signed vorticity, a locally peaked secondary vorticity is induced on the latter sheet. This emerging secondary vorticity results in a remarkable vorticity amplification on the stronger sheet, forming pseudo vortex pairs.

## [04164] Compressible Kelvin-Helmholtz and Rayleigh-Taylor Instabilities

**Author(s)** : Yasuhide Fukumoto (Kyushu University)Rong Zou (Zhejiang Normal University)Kazuo Matsuura (Ehime University)Nobutaka Taniguchi (University of Tokyo)

**Abstract** : For an incompressible fluid, an interface of tangential-velocity discontinuity suffers from the Kelvin-Helmholtz instability (KHI), with growth rate proportional to velocity discontinuity. Compressibility acts to stabilize KHI and, if limited to two dimensions, suppresses KHI for the Mach number larger than  $\sqrt{8}$ . We extend this analysis to include the gravity effect, with allowance made for density discontinuity and surface tension. Numerical simulations of a compressible mixing layer, being desingularization, exhibit complex vortical structures in turbulence.

02578 (3/4) : 2D @G704

## [04478] Compressible Vortex Sheets and Free Boundary Problems

**Author(s)** : Gui-Qiang George Chen (University of Oxford)

**Abstract** : We are concerned with the nonlinear stability/instability of compressible vortex sheets and related interfaces in compressible fluid flows governed by the Euler equations and related nonlinear PDEs. Such problems can be formulated as characteristic free boundary problems for nonlinear hyperbolic conservation laws and related equations. In this talk, we will discuss some recent developments in the analysis of their stability/instability and explore stabilizing mechanisms such as magnetic, relativistic, and compressibility effects.

## [04545] Special self-similar class in Rayleigh-Taylor interfacial mixing

**Author(s)** : Snezhana Abarzhi (University of Western Australia)

**Abstract** : Rayleigh-Taylor mixing governs a broad range of processes in nature and technology. We discover special self-similar class in Rayleigh-Taylor mixing with variable accelerations, by exploring its symmetries, scaling laws, correlations and fluctuations. We find that Rayleigh-Taylor mixing can vary from super-ballistics to sub-diffusion depending on the acceleration and retain memory of deterministic conditions for any acceleration. We explain high Reynolds number experiments in Rayleigh-Taylor mixing and provide new insights for processes driven by the mixing.

## [04546] Interface dynamics in ideal and realistic fluids

**Author(s)** : Dan V. Ilyin (California Institute of Technology)Snezhana Abarzhi (University of Western Australia)

**Abstract** : Interfaces and mixing and their non-equilibrium dynamics are ubiquitous to occur in nature and technology. We develop theory of interface dynamics, directly linking flow fields and interfacial transport and discovering fluid instabilities never previously discussed. In ideal and realistic fluids, the interface stability is set by

the interplay of the macroscopic inertial mechanism balancing the destabilizing acceleration, whereas microscopic thermodynamics create vortical fields in the bulk. The interface is the place where balances are achieved.

## [05008] Generalized Ideal Momentum Jet Model for Non-Circular Nozzle Geometries in Turbulent Pressure-Atomized Liquid Jets: Theoretical and Experimental Comparison

**Author(s)** : Fermin Franco-Medrano (Autonomous University of Baja California)

**Abstract** : We propose a generalized mathematical model for turbulent pressure-atomized liquid jets with non-circular nozzles and compare to experimental data. We obtain analytical expressions for the locally homogeneous two-phase flow properties as a function of gauge pressure, nozzle dimensions, and fluid densities. Interestingly, we find that the equations describing elliptical and rectangular nozzles are generalizations of those for circular nozzles. Strong correlation is observed between the experimental data and our model function for the elliptical nozzle jet velocity.

02578 (4/4) : 2E @G704

## [05070] A novel data analysis method for Rayleigh-Taylor mixing

**Author(s)** : Kurt Christian Williams (The University of Western Australia)Snezhana Abarzhi (University of Western Australia)

**Abstract** : A recent data analysis method has shed new light on the isotropy and dynamics of Rayleigh-Taylor mixing; the late-stage behavior of two fluids accelerated against their density gradient. In this talk, we elaborate this data analysis method, which employs Whittle estimates based on a new goodness-of-fit test statistic generated from Monte-Carlo methods. Employing a fitting function from isotropic turbulence, the method finds the isotropy of Rayleigh-Taylor mixing and captures a broad dynamic range.

## [02591] Recent advances in data-driven modeling and computational methods

**Session Time & Room :**

02591 (1/2) : 5C (Aug.25, 13:20-15:00) @G301

02591 (2/2) : 5D (Aug.25, 15:30-17:10) @G301

**Type** : Proposal of Minisymposium

**Abstract** : The minisymposium "recent advances in data-driven modeling and computational methods" covers a wide range of topics including topological data analysis, physics-informed neural networks, and data-driven modeling and numerical methods. It provides a platform for experts and junior researchers to exchange ideas and share knowledge in these areas.

This minisymposium is organized by the East Asia section of SIAM (EASIAM), and the organizers and speakers represent a broad list of countries covered by SIAM. We hope the minisymposium would provide an ideal opportunity for communication among EASIAM members, and to promote EASIAM internationally.

**Organizer(s)** : Yoshinobu Kawahara, Yao Yao, Zhiwen Zhang

**Classification** : 00A69, 00A71

**Minisymposium Program :**

02591 (1/2) : 5C @G301 [Chair: Yang Xiang]

## [02896] Topological Data Analysis Experience in Malaysia: A Survey

**Format** : Talk at Waseda University

**Author(s)** : Fatimah Abdul Razak (Universiti Kebangsaan Malaysia)Mohd Salmi Md Noorani (Universiti Kebangsaan Malaysia)

**Abstract** : Topological Data Analysis (TDA) is used to detect qualitative features in datasets. It is often combined

with techniques from Machine Learning, Time Series Analysis as well as Complex Network Analysis to achieve better predictions and classifications. This presentation outlines our experiences of using TDA to investigate several Malaysian data sets in order to predict floods and financial crises, classify different levels of air quality within a certain time window as well as detecting critical transitions.

## [03038] A Reaction Network Analysis of Insulin Signaling

**Format :** Talk at Waseda University

**Author(s) :** Angelyn Lao (De La Salle University)

**Abstract :** The insulin signaling system is an important metabolic system that initiates the uptake of glucose into the cell. This reduced ability of cells to use available insulin for energy metabolism is viewed as a common factor in diseases such as obesity, type 2 diabetes, metabolic syndrome, and cancer, and more recently to brain insulin resistance in connection with mild cognitive impairment and Alzheimer's disease (AD). The complexity of the insulin signaling system, both in terms of the number of molecular components involved as well as the intricate combination of positive and negative feedback loops, clearly warrants the application of mathematical modeling and computational tools. This talk presents the construction of the insulin signaling reaction network and the analysis of its robustness and stability using Chemical Reaction Network Theory.

## [03583] Comparing Lagrangian Particle Dispersion Models in Turbulent Flows: A Data-Driven Approach

**Format :** Talk at Waseda University

**Author(s) :** Nurul Huda Mohd Ramli (Universiti Brunei Darussalam) Haziq Jamil (Universiti Brunei Darussalam)

**Abstract :** This talk introduces a data-driven method for comparing two Lagrangian stochastic particle models in turbulent flows: the random flight model (RFM) and the simpler random displacement model (RDM). The RFM offers a more realistic representation of eddy velocities but can pose computational challenges. Using a Bayesian approach to infer the models' parameters, the objective is to provide a better understanding of their dynamics and assist researchers in selecting the appropriate model for their specific needs.

## [03912] Error estimates of numerical methods for the Dirac equation

**Format :** Talk at Waseda University

**Author(s) :** Ying Ma (Beijing University of Technology) Jia Yin (Lawrence Berkeley National Laboratory) Yue Feng (Sorbonne Université) Lizhen Chen (Beijing Computational Science Research Center)

**Abstract :** The Dirac equation is a relativistic wave equation which plays an important role in relativistic quantum physics and provides a natural description of relativistic spin-1/2 particles. In this talk, we present numerical methods including several finite difference methods, the symmetric and asymmetric exponential wave integrator Fourier pseudospectral methods and establish the error estimates for the discretization of the Dirac equation in different regimes. Extensive numerical results are reported to support our error estimates.

02591 (2/2) : 5D @G301 [Chair: Tao Zhou]

## [04021] A learning-based projection method for model order reduction of transport problems

**Format :** Talk at Waseda University

**Author(s) :** ZHICHAO PENG (Hong Kong University of Science and Technology) Fengyan Li (Rensselaer Polytechnic Institute) Min Wang (University of Houston)

**Abstract :** Due to the slow decay of the Kolmogorov n-width for transport problems, classical linear reduced order model (ROM) may be inefficient. To address this issue we propose a learning-based projection method following an offline-online decomposition framework. A moving low dimensional subspace is learned offline, and in the online stage, the full order problem is projected onto the learned subspace to reduce computational cost. We also numerically demonstrate the performance of the proposed method.

## [04197] An iterative algorithm for POD basis adaptation

**Format :** Talk at Waseda University

**Author(s) :** Zhizhang Wu (The University of Hong Kong) Zhiwen Zhang (The University of Hong Kong)

**Abstract :** To construct reduced-order models using POD for convection-diffusion equations, fine-grid solvers are needed to obtain accurate solution snapshots for small diffusivities, while coarse-grid solvers are sufficient for large diffusivities. We develop an iterative algorithm that adapts the POD basis functions extracted at large diffusivities

part\_2

for the construction of reduced-order models at small diffusivities without resorting to fine-grid solvers. Convergence analysis and numerical results are provided to confirm the effectiveness of our method.

## [04384] Heat on hypergraph and its application to network analysis

**Format :** Talk at Waseda University

**Author(s) :** Masahiro Ikeda (RIKEN)

**Abstract :** In this talk, I will introduce the joint works with Atsushi Miyauchi (Tokyo Univ.), Yuuki Takai(KIT) and Yuichi Yoshida (NII). They are about heat on hypergraph and its application to network analysis. I will introduce the background of their papers and the fundamental notions for community detection of networks. First I review the notion of Laplacian and Cheeger's inequality for the usual undirected graph. After that, I introduce the definition of the (submodular) Laplacian for hypergraphs and the heat on them. I also introduce several properties of the Laplacian and heat such as maximal monotonicity of the Laplacian. Especially I explain well-definedness of the heat and the Personalized PageRank for hypergraphs. Moreover, I introduce applications of their properties to the community detection on hypergraphs. If time permitted, I will introduce recent works about submodular Laplacian with Uchida (Oita Univ.).

## [04987] Convergence Rate Analysis for Deep Ritz Method

**Format :** Talk at Waseda University

**Author(s) :** Jerry Zhijian Yang (Wuhan University)

**Abstract :** We provide a rigorous numerical analysis on deep Ritz method (DRM) for second order elliptic equations with Neumann boundary conditions. We establish the first nonasymptotic convergence rate in  $H^1$  norm for DRM using deep networks with ReLU2 activation functions. Our study also shed light on how to set the hyperparameter of depth and width to achieve the desired convergence rate in terms of number of training samples.

# [02600] Applied and computational discrete algorithms

**Session Time & Room :**

02600 (1/2) : 3D (Aug.23, 15:30-17:10) @G404

02600 (2/2) : 3E (Aug.23, 17:40-19:20) @G404

**Type :** Proposal of Minisymposium

**Abstract :** Combinatorial and discrete mathematical problems arise in many real-life applications. Their solution requires designing, analyzing and implementing discrete algorithms. The research in this area therefore brings together mathematicians, computer scientists, statisticians, domain scientists and engineers to solve problems of applied and computational combinatorics. The proposed two-part minisymposium covers scientific computing, machine learning, and graph algorithms. The objective is to summarize the latest discrete algorithmic developments and their applications with computational studies on the applications. This minisymposium follows similar ones held in ICIAM 2019, ICIAM 2015, and ICIAM 2011 on combinatorial aspects of sparse matrix computations.

**Organizer(s) :** Alex Pothen, Bora Ucar

**Classification :** 05C85, 65F50, 68W05

**Minisymposium Program :**

02600 (1/2) : 3D @G404 [Chair: Bora Ucar]

## [04306] Parallel Batch-Dynamic Graph Algorithms

**Format :** Online Talk on Zoom

**Author(s) :** Julian Shun (MIT)

**Abstract :** There has been significant interest in graph analytics due to their applications in many domains, including social network and Web analytics, machine learning, biology, and physical simulations. Real-world graphs today are massive and also dynamic. As many real-world graphs change rapidly, it is crucial to design

dynamic algorithms that efficiently maintain graph statistics upon updates, since the cost of re-computation from scratch can be prohibitive. Furthermore, due to the high frequency of updates, we can improve performance by using parallelism to process batches of updates at a time. This talk presents new graph algorithms in this parallel batch-dynamic setting.

Specifically, we present the first parallel batch-dynamic algorithm for approximate k-core decomposition that is efficient in both theory and practice. Our algorithm is based on our novel parallel level data structure, inspired by the sequential level data structures of Bhattacharya et al. and Henzinger et al. Given a graph with  $n$  vertices and a batch of  $B$  updates, our algorithm maintains a  $(2 + \epsilon)$ -approximation of the coreness values of all vertices (for any constant  $\epsilon > 0$ ) in  $O(B \log^2(n))$  amortized work and  $O(\log^2(n) \log\log(n))$  span (parallel time) with high probability. We implement and experimentally evaluate our algorithm, and demonstrate significant speedups over state-of-the-art serial and parallel implementations for dynamic k-core decomposition.

We have also designed new parallel batch-dynamic algorithms for low out-degree orientation, maximal matching, clique counting, graph coloring, minimum spanning forest, single-linkage clustering, some of which use our parallel level data structure.

## [03109] Approximation: a Paradigm for Designing Parallel Graph Algorithms

**Format :** Online Talk on Zoom

**Author(s) :** Alex Pothen (Purdue University )S M Ferdous (Pacific Northwest National Lab )

**Abstract :** We describe a paradigm for designing parallel algorithms by approximation techniques. Instead of solving a problem exactly, for which parallel algorithms may not exist, we seek a solution with provable approximation guarantees. Furthermore, we design these algorithms to be concurrent. We discuss linear and submodular matching and edge cover problems for which such algorithms have been designed, and describe their use in solving problems in sparse matrix computations and load balancing problems in quantum chemistry.

## [02991] Nested dissection ordering on GPUs

**Format :** Talk at Waseda University

**Author(s) :** Xiaoye Sherry Li (Lawrence Berkeley National Lab)

**Abstract :** Nested dissection ordering is an important preprocessing step in sparse matrix factorizations. It is effective in reducing the amount of fill in the factored matrices.

As of now, there is no good algorithm nor software to compute such an ordering on GPUs. We have made some progress in this direction.

We will present our new algorithms designed for GPUs, including multilevel graph coarsening and finding small separators at each level, and the results of parallel runtime and ordering quality.

## [05454] Accelerating AI using Fast and Feasible Matrix Multiplication

**Format :** Online Talk on Zoom

**Author(s) :** Oded Schwartz (The Hebrew University)

**Abstract :** AI requires large resources, both for training and for inference. It involves significant time spent on matrix multiplication, typically between 45%-95%. Most current math libraries (for CPU and GPU) and all state-of-the-art hardware accelerators (such as Google's TPU and Intel's / Habana Lab's Gaudi) are based on the cubic-time classic matrix multiplication algorithm, despite more than five decades of research on sub-cubic time algorithms. In this talk I will review several of the challenges in utilizing fast matrix multiplication algorithms, and recent solutions that can allow faster application in practice.

02600 (2/2) : 3E @G404 [Chair: X. Sherry Li]

## [03099] On heuristics for the Birkhoff--von Neumann decomposition

**Format :** Online Talk on Zoom

**Author(s) :** Bora Ucar (CNRS and ENS de Lyon)Jeremy Cohen (CREATIS, CNRS)

**Abstract :** The Birkhoff--von Neumann decomposition expresses a doubly stochastic matrix as a convex combination of permutation matrices. This talk will be an introduction to this decomposition. We will discuss algorithmic and combinatorial problems associated with this decomposition.

## [03435] Recent Advances in Streaming (Hyper)Graph Partitioning

**Format :** Online Talk on Zoom

**Author(s) :** Christian Schulz (Heidelberg University)

**Abstract :** Partitioning a (hyper)graph into balanced blocks such that few edges run between blocks is a key problem for large-scale distributed processing.

Currently there is a gap observed in the space of available partitioning algorithms. On the one hand, there are streaming algorithms that have been adopted to partition massive graph data on small machines. In the streaming model, vertices arrive one at a time including their neighborhood and then have to be assigned directly to a block. These algorithms can partition huge graphs quickly with little memory, but they produce partitions with low solution quality. On the other hand, there are offline (shared-memory) multilevel algorithms that produce partitions with high quality but also need a machine with enough memory to partition huge networks.

In this talk, we present recent advances in the area of streaming algorithms for the problem. First, we present a buffered streaming approach: this model allows to read more than one node and its neighborhood at the time. This enables our algorithm to leverage multilevel techniques, and thus significantly improve solution quality while surprisingly also enhancing the overall complexity of the algorithm.

On the other hand, we present a shared-memory streaming multi-recursive partitioning scheme that performs recursive multi-sections on the fly without knowing the overall input graph to compute hierarchical partitionings. If the topology of a distributed system is known, it is possible to further optimize the communication costs by mapping partitions onto processing elements.

## [04746] Efficient Data Structures for Sparse Dynamic Graphs

**Format :** Talk at Waseda University

**Author(s) :** Helen Xu (Lawrence Berkeley National Laboratory)

**Abstract :** Sparse graphs underlie many key applications such as social networks analyses and scientific computing. This talk discusses dynamic graph data structures and how to choose data structures that optimize for locality, which is key to performance in graph computations. The focus is on how different use cases, which can cause different data patterns and access patterns, can influence the design of these structures and how to exploit these differences to maximize performance.

## [04669] Communication Efficient Stratified SGD on Distributed-Memory Systems

**Format :** Online Talk on Zoom

**Author(s) :** Nabil Abubaker (Bilkent University) Ozan Karsavuran (Lawrence Berkeley National Lab) Cevdet Aykanat (Bilkent University)

**Abstract :** Stratified Stochastic Gradient Descent (SSGD) enables stale-free low-rank approximation of sparse matrices on distributed-memory systems. We present a framework to efficiently scale SSGD on HPC systems. The framework leverages point-to-point communications to reduce the bandwidth overhead, and a novel combinatorial algorithm to reduce the upper bound on the number of messages from  $O(K^2)$  to  $O(K \log K)$ , where  $K$  is the number of processors. Our experiments show an order of magnitude performance gap in favor of our framework-enabled SSGD compared to the state-of-the-art.

## [02612] Mathematical modeling of biofilm systems and applications

**Session Time & Room :**

02612 (1/2) : 4C (Aug.24, 13:20-15:00) @D514

02612 (2/2) : 4D (Aug.24, 15:30-17:10) @D514

**Type :** Proposal of Minisymposium

**Abstract :** The majority of microbial life on Earth occurs in biofilms, heterogeneous microbial communities embedded in layers of a self-produced extracellular matrix. Biofilms have a detrimental role in industrial and medical applications, via antibiotic-resistant infections, corrosion and fouling. On the other hand, they are also widely used in bioremediation technologies to improve water quality and generate renewable resources. The non-

part\_2

linear, multidimensional and multiscale nature of these complex microbial systems provides ample opportunity for investigation with theoretical modeling. This minisymposium focuses on continuum deterministic models, and brings together different biofilm applications, modeling approaches, and methods for model analysis.

**Organizer(s)** : N.G. Cogan, Vincenzo Luongo, Maria Rosaria Mattei

**Classification** : 92Bxx, 35QXX

**Minisymposium Program :**

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02612 (1/2) : 4C @D514

## [03848] Simulation of ultrasonic biofilm detachment in membrane aerated bioreactors

**Author(s)** : Maryam Ghasemi (University of Waterloo)Sheng Chang (University of Guelph)Sivalaban Sivaloganathan (University of Waterloo)

**Abstract** : Controlling biofilm thickness in an aerated membrane biofilm reactor (MBfR) has been recognized as a key for MBfRs to achieve a long-term stable performance. In this context, acoustic cavitation is an effective strategy that can be used for controlling biofilm thickness. However, to maintain the biofilm thickness at an optimum value, it is necessary to understand the effect of acoustic parameters and cavitation bubble distribution on biofilm detachment and establish a link between biofilm detachment and regrowth. The purpose of this study is to provide an integrated mathematical model that describes biofilm development in an aerated membrane biofilm reactor using a nonlinear reaction-diffusion model and its response to mechanical stress generated from acoustic cavitation. The simulation results show that amplitude and frequency of transducer are two key factors that affect biofilm detachment. Moreover, uniform distribution of cavitation along the biofilm surface is critical to achieve an even biofilm thickness. Furthermore, periodic cavitation detachment with an appropriate resting time in between is important for maintaining the biofilm thickness at a desired value. Therefore, the proposed integrated modeling approach can be used to optimize acoustic cavitation parameters and achieve effective biofilm thickness control in MBfRs.

## [04151] Bacterial Biofilms across scales and applications

**Format** : Online Talk on Zoom

**Author(s)** : Nicholas Cogan (Florida State University)

**Abstract** : This talk will describe mathematical modeling of biofilm dynamics in general. This should set the stage for the talks in this session that include models that focus on the physics of fluids, materials, and biology. Applications range from environmental to engineering as well as scales from millimeters to meters and time scales that range from seconds to weeks. Because of the wide variety in scales and applications, mathematical aspects must be both flexible and precise. This tension has driven an explosion in interest in biofilm models in the past 30+ years and there are a handful of broadly studied models which will be discussed in this talk.

## [04177] Microbially-influenced transport in sea ice

**Author(s)** : Isaac Klapper (Temple University)

**Abstract** : Sea ice, which covers a significant portion of the earth's surface, is an interestingly complicated material consisting of a mixture of solid ice and liquid brine phases which are coupled by thermodynamic considerations. It also is a platform for microbial life. A model will be presented that hypothesizes that, in turn, the sea ice resident microbial population

might impact ice sheet structure and, in particular, its transport properties including notably heat transport.

## [04844] Computational simulations of biofouling on ship hulls

**Author(s)** : Rosalind Allen (Friedrich Schiller University Jena)Patrick Sinclair (University of Edinburgh)Jennifer Longyear (AkzoNobel)Kevin Reynolds (AkzoNobel)Alistair Finnie (AkzoNobel)Chris Brackley (University of Edinburgh)Martin Carballo Pacheco (University of Edinburgh)

**Abstract** : We use computer simulations to investigate two coating technologies for ship hulls. Simulating microbial colonization of a surface that releases a biocidal chemical we find intrinsic stochasticity with an important role for immigration of biocide-resistant species. Further, computational fluid dynamics simulations of flow across a textured (riblet) surface show that removal of biofouling by flow may be ineffective if the flow is not well aligned. Simulations can help understand marine biofouling on advanced surface coatings.

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02612 (2/2) : 4D @D514

## [05492] Long time behaviour of a thin-film model for early biofilm development

**Author(s)** : John Ward (Loughborough University)

**Abstract** : We will present a model describing the interaction of a thin, surface growing biofilm and planktonic cells. Assuming the biofilm can be described as homogeneous, thin, highly viscous fluid, a coupled system of nonlinear reaction-diffusion equations is derived, one of which having a fourth-order "diffusion" term. Key results using numerical computation and asymptotic analysis will be presented that indicate the dominant processes in early biofilm expansion and the subtle complexities of the travelling wave solutions.

## [02613] Advances in Variational and Hemivariational Inequalities: Modeling, Analysis, and Applications

**Session Time & Room :**

02613 (1/3) : 5B (Aug.25, 10:40-12:20) @G606

02613 (2/3) : 5C (Aug.25, 13:20-15:00) @G606

02613 (3/3) : 5D (Aug.25, 15:30-17:10) @G606

**Type** : Proposal of Minisymposium

**Abstract** : This minisymposium highlights recent developments in the mathematical analysis, numerical solution, and real-world applications of variational and hemivariational inequalities. The focus is on the modeling of problems leading to such inequalities, the well-posedness and properties of their solutions, numerical analysis, optimal control and optimization, and their applications in mechanics and physics. The related topics include, but are not limited to, dynamical systems, fixed points, nonconvex and nonsmooth analysis, nonlinear inclusions, and numerical methods. The overall goal of the minisymposium is to foster collaboration and knowledge-sharing among researchers working in the area of variational and hemivariational inequalities and their applications.

**Organizer(s)** : Stanislaw Migorski, Fei Wang

**Classification** : 35L87, 47J20, 49J52, 65K15, 65N30

**Minisymposium Program :**

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02613 (1/3) : 5B @G606 [Chair: Fei Wang]

## [04082] Recent Advances on Partial Differential Variational Inequalities

**Format** : Talk at Waseda University

**Author(s)** : zhenhai Liu (guangxi minzu university)

**Abstract** : In this talk, we consider a partial differential complex system obtained by mixing an evolution partial differential equation and a variational inequality. This kind of problems may be regarded as a special feedback control problem. Firstly, we give our research motivation and examples. Then, based on the theory of semigroups, Filippov implicit function lemma and fixed point theory for set-valued mappings, we show several existence results of solutions to the mentioned problem. Finally we point out some problems for the further research.

## [03283] Optimal control for variational inequalities of obstacle type

**Format** : Talk at Waseda University

**Author(s)** : Zijia Peng (Guangxi Minzu University)

**Abstract** : This talk is concerned with optimal control of obstacle problems whose weak formulations are nonlinear variational inequalities. Under appropriate assumptions, existence of optimal solutions is proved. Moreover, the necessary optimality conditions of first order are derived by regularization techniques.

## [03248] Approximation techniques for solving hemivariational inequalities arising from contact mechanics

**Format :** Talk at Waseda University

**Author(s) :** Li Zhibao (Central South University)

**Abstract :** Frictional contact phenomena are common in various industrial processes and engineering applications, and they can be described by variational or hemivariational inequalities. Most of these inequality problems lack analytical solutions. Hence, developing effective numerical methods to solve these inequalities is important. Hemivariational inequality is a useful tool to study nonlinear boundary value problems with nonsmooth and nonconvex functionals. With finite element discretization, HVIs become nonconvex optimization problems. In this talk, I will present some numerical methods based on approximation techniques to solve the nonconvex optimization problem for the hemivariational inequality arising from the frictional contact mechanics problem. These methods include the smooth quadratic regularization method, as well as the first and second order approximation methods for the nonconvex functions. I will also evaluate and compare these methods using numerical experiments at the end.

## [03265] A virtual element method for a quasistatic frictional contact problem

**Format :** Talk at Waseda University

**Author(s) :** fang feng (East China Normal University )Weimin Han (University of Iowa)Jianguo Huang (Shanghai Jiao Tong University)

**Abstract :** We consider the numerical solution of an abstract quasistatic variational inequality arising in the study of quasistatic physical processes. The temporal discretization is carried out by the backward difference method, while the spatial discretization is based on the virtual element method. A general framework is provided and a quasistatic contact problem is studied and the optimal order error estimates are derived for the lowest-order virtual element method.

02613 (2/3) : 5C @G606 [Chair: Zhenhai Liu]

## [04032] The interior penalty virtual element method for the fourth-order elliptic hemivariational inequality

**Format :** Talk at Waseda University

**Author(s) :** Jiali Qiu (Xi'an Jiaotong University)Fei Wang (Xi'an Jiaotong University)Min Ling (School of Mathematical Sciences, Peking University)Jikun Zhao (Zhengzhou University)

**Abstract :** We develop the interior penalty virtual element method (IPVEM) for solving a Kirchhoff plate contact problem, which can be described by a fourth-order elliptic hemivariational inequality (HVI). With certain assumptions, the well-posedness of the discrete problem is proved. Furthermore, a priori error estimation is established for the IPVEM for the fourth-order elliptic HVI, and we show that the lowest-order VEM achieves optimal convergence order. Finally, some numerical examples are presented to support the theoretical results.

## [03325] Virtual element method for a frictional contact problem with normal compliance

**Format :** Talk at Waseda University

**Author(s) :** Bangmin Wu (Xinjiang University)

**Abstract :** We study the virtual element method for solving the frictional contact problem with the normal compliance condition, which can be modeled by a quasi-variational inequality. Existence and uniqueness results are obtained for the discretized scheme. Furthermore, a priori error analysis is established, and an optimal order error bound is derived for the lowest order virtual element method. One numerical example is given to show the efficiency of the method and to illustrate the theoretical error estimate.

## [03328] Well-posedness and Numerical Analysis of a Stokes Hemivariational Inequality

**Format :** Online Talk on Zoom

**Author(s) :** Min Ling (School of Mathematical Sciences, Peking University)

**Abstract :** This talk is devoted to the development and analysis of a pressure projection stabilized mixed finite element method, with continuous piecewise linear approximations of velocities and pressures, for solving a hemivariational inequality of the stationary Stokes equations with a nonlinear non-monotone slip boundary condition. We present an existence result for an abstract mixed hemivariational inequality and apply it for a unique solvability analysis of the numerical method for the Stokes hemivariational inequality. An optimal order error estimate is derived for the numerical solution under appropriate solution regularity assumptions. Numerical results are presented to illustrate the theoretical prediction of the convergence order.

## [03157] Well-posedness of parabolic variational-hemivariational inequalities with unilateral constraints

**Format :** Online Talk on Zoom

**Author(s) :** Stanislaw Migorski (Jagiellonian University in Krakow)Dong-ling Cai (School of Mathematical Sciences, University of Electronic Science and Technology of China)

**Abstract :** In this talk we discuss a novel class of variational-hemivariational inequalities with a unilateral constraint of parabolic type. Results on existence, uniqueness and the continuous dependence of the weak solution with respect to perturbations in the data are proved. As an application we examine a mathematical model of nonsmooth quasistatic viscoelastic frictional contact problem with the Signorini unilateral contact condition and a generalization of the static Coulomb law of dry friction.

02613 (3/3) : 5D @G606 [Chair: Stanislaw Migorski]

## [03234] Duality Arguments in Analysis of Viscoelastic Contact Problem

**Format :** Online Talk on Zoom

**Author(s) :** Anna Ochal (Jagiellonian University in Krakow)

**Abstract :** We consider a mathematical model which describes the quasistatic frictionless contact of a viscoelastic body with a rigid-plastic foundation. We provide three different variational formulation of the model in which the unknowns are the displacement, the stress and the strain, respectively. We prove that they are pairwise dual of each other and they are well-posedness. The proofs are based on recent results on history-dependent variational inequalities and inclusions.

## [03636] Frictional contact problem for electrorheological fluid flows

**Format :** Online Talk on Zoom

**Author(s) :** Dariusz Pączka ( Warsaw University of Technology)

**Abstract :** We study the stationary flow of an isothermal, homogeneous and incompressible electrorheological fluid with slip boundary conditions of frictional type. The variational formulation of the flow problem has the form of a hemivariational inequality. Existence and uniqueness of a weak solution to the hemivariational inequality is proved for a material function  $p(\cdot)$  of an electric field without any condition of monotonicity type on the extra stress tensor. This result is established by abstract theorems on existence and uniqueness of a solution to a subdifferential operator inclusion and a hemivariational inequality in the variable exponent Sobolev space.

## [03327] Numerical analysis of history-dependent variational-hemivariational inequality by virtual element method

**Format :** Online Talk on Zoom

**Author(s) :** Wenqiang Xiao (School of Mathematical Sciences, Peking University)

**Abstract :** In this talk, we mainly introduce the virtual element method for solving two types of history-dependent variational-hemivariational inequalities arising in contact problems. In the first model, we consider an elastic material. The contact is modelled with a total slip-dependent version of Coulomb's law of dry friction. In the second model, we consider viscoelastic material. We introduce fully discrete schemes for the above two problems,

where the temporal integration is approximated by trapezoidal rule and the spatial variable is approximated by the virtual element methods. An optimal order error estimates is derived under appropriate solution regularity assumptions. Finally, numerical examples are reported, providing numerical evidence of the optimal convergence order theoretically predicted.

## [03250] Stability analysis for nonstationary Stokes hemivariational inequality

**Format :** Online Talk on Zoom

**Author(s) :** Changjie Fang (Chongqing University of Posts and Telecommunications)

**Abstract :** In this talk, we consider hemivariational inequality problem for the evolutionary Stokes equations with a nonlinear slip boundary condition. We assume the slip boundary condition together with a Clarke subdifferential relation between the stress tensor and velocity. The existence of weak solutions is obtained by Galerkin method. In addition, stability is analyzed for a perturbed hemivariational inequality. We also present a result on the existence of a solution to an optimal control problem for the nonstationary Stokes hemivariational inequality

## [02616] Recent Developments in Applied Inverse Problems

**Session Time & Room :**

02616 (1/3) : 1C (Aug.21, 13:20-15:00) @G808

02616 (2/3) : 1D (Aug.21, 15:30-17:10) @G808

02616 (3/3) : 1E (Aug.21, 17:40-19:20) @G808

**Type :** Proposal of Minisymposium

**Abstract :** This minisymposium addresses both theoretical and algorithmic aspects of inverse problems arising in tomography as well as their applications. We will bring together well established scientists and young researchers to provide a forum to discuss new ideas and developments in the field of applied inverse problems.

**Organizer(s) :** Hiroshi Fujiwara, Kamran Sadiq

**Classification :** 35R30, 65Nxx, 74Jxx, 78Axx, 45Exx

**Minisymposium Program :**

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02616 (1/3) : 1C @G808 [Chair: Kamran Sadiq]

## [04397] Perturbation of Surface Waves in Piezoelectric Media

**Format :** Talk at Waseda University

**Author(s) :** Kazumi Tanuma (Gunma University)Xiang Xu (Zhejiang University)Gen Nakamura (Hokkaido University)

**Abstract :** We study Bleustein-Gulyaev (BG) waves which propagate along the surface of a homogeneous  $C_6$  hexagonal piezoelectric half-space under the mechanically-free and electrically-closed condition at the surface. We prove stability of the BG waves, to investigate the perturbations of their phase velocity and polarization when a fully anisotropic perturbation is added to the hexagonal material constants. The inverse problem to obtain material information from measurements of BG waves will be discussed.

## [04646] Quantitative Parameter Reconstruction from Optical Coherence Tomographic Data

**Format :** Talk at Waseda University

**Author(s) :** Leopold Veselka (University of Vienna)

**Abstract :** We discuss the quantification of the refractive index from data obtained by optical coherence tomography - an imaging modality based on the interferometric measurement of back-scattered light. We consider samples with layered structure, where the refractive index as a function of depth is a piece-wise constant function. The applicability of the reconstruction method, where the refractive index is obtained layer-by-layer via least squares minimization, is verified by numerical examples for both simulated and experimental data.

This is a joint work with Peter Elbau (University of Vienna, Austria) and Leonidas Mindrinos (Agricultural University of Athens, Greece).

## [04241] Landweber-Kaczmarz for full datacube modelling in Extragalactic Archaeology

**Format :** Talk at Waseda University

**Author(s) :** Fabian Hinterer (JKU Linz)

**Abstract :** We consider the problem of reconstructing a galaxy's stellar population distribution function from spectroscopy measurements. These quantities can be connected via the single-star population spectrum, resulting in a very large scale integral equation with a system structure. To solve this problem, we propose a projected Nesterov-Kaczmarz reconstruction (PNKR) method, which efficiently leverages the system structure and incorporates physical prior information such as smoothness and non-negativity constraints.

02616 (2/3) : 1D @G808 [Chair: Hiroshi Fujiwara]

## [03014] Principles and Examples of Magnetic Resonance Elastography for Distribution Measurement of Viscoelasticity

**Format :** Talk at Waseda University

**Author(s) :** Mikio Suga (Chiba University)

**Abstract :** The mechanical property of a tissue is related to physiological and pathological states. Magnetic resonance elastography (MRE) is an imaging technique that can noninvasively measure the physical properties of biological soft tissues by using a magnetic resonance imaging system. Measuring the mechanical properties of tissues is expected to be helpful in diagnosing diseases such as hepatic fibrosis and cancer. In this minisymposium, I will talk about the principles and examples of MRE.

## [04180] Inverse scattering technique for a defect in anisotropic plates

**Format :** Talk at Waseda University

**Author(s) :** Takahiro SAITO (Gunma University)

**Abstract :** In recent years, plates with anisotropic properties, such as CFRP, have been increasingly used in the engineering industry. In general, it is known that the elastic wave propagation is very complicated in anisotropic plates, due to the anisotropic properties and the generation of some types of wave modes between the incident wave and both upper and lower surfaces. In this study, the author proposes an inverse scattering technique for reconstructing a defect in anisotropic plates.

02616 (3/3) : 1E @G808 [Chair: Hiroshi Fujiwara]

## [03045] Source Reconstruction from Partial Boundary Data in Radiative Transport

**Format :** Talk at Waseda University

**Author(s) :** Kamran Sadiq (Johann Radon Institute for Computational and Applied Mathematics (RICAM))

**Abstract :** This talk concerns the source reconstruction problem in a transport problem through an absorbing and scattering medium from boundary measurement data on an arc of the boundary. The method, specific to two dimensional domains, relies on Bukhgeim's theory of A-analytic maps and it is joint work with A. Tamasan (UCF) and H. Fujiwara (Kyoto U).

## [03961] Numerical challenges to optical tomography by the stationary radiative transport equation

**Format :** Talk at Waseda University

**Author(s) :** I-Kun Chen (National Taiwan University) Hiroshi Fujiwara (Kyoto University) Daisuke Kawagoe (Kyoto University)

**Abstract :** We discuss quantitative feasibility of optical tomography based on the stationary radiative transport equation which is a mathematical model of particle migration with absorption and scattering by medium. The key idea is the use of discontinuity of its solution induced by a proper boundary condition and discontinuous Galerkin

methods. Numerical examples are exhibit to show a possibility of reconstruction of the attenuation coefficient without a priori information on the scattering kernel.

## [04301] Inversion of the momenta X-ray transform of symmetric tensor fields in the plane.

**Format :** Online Talk on Zoom

**Author(s) :** Alexandru Tamasan (University of Central Florida)Kamran Sadiq (Johann Radon Institute for Computational and Applied Mathematics (RICAM))David Omogbhe (University of Vienna)Hiroshi Fujiwara (Kyoto University)

**Abstract :** The X-ray transform of symmetric tensor fields recovers the tensor field only up to a potential field. In 1994,

V. Sharafutdinov showed that augmenting the X-ray data with several momentum  $X$ -ray transforms establishes uniqueness, with a most recent work (2022) showing stability of the inversion. In this talk, I will present a first reconstruction method, which stably recovers sufficiently smooth symmetric tensor fields compactly supported in the plane.

The method is based on the extension of Bukhgeim's theory to a system of A-analytic maps. This is joint work with H. Fujiwara, D. Omogbhe and K. Sadiq.

## [02618] Recent Developments in Hyperspectral and Multispectral Imaging

**Session Time & Room :** 5C (Aug.25, 13:20-15:00) @E605

**Type :** Proposal of Minisymposium

**Abstract :** Hyperspectral and multispectral images contain plenties of spatial-spectral information, which brings a substantial opportunity to explore and understand their features. This Mini-symposium provides a platform for researchers to share innovative ideas about algorithm developments associated with this type of imaging. Attendees can expect to learn about the latest techniques from model-based and data-driven perspectives and their applications in remote sensing, computational imaging, and medical imaging.

**Organizer(s) :** Chao Wang, Jizhou Li

**Classification :** 65K10, 68U10, 49N45

**Minisymposium Program :**

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02618 (1/1) : 5C @E605 [Chair: Chao Wang]

## [03524] Multi-Dimensional Signal Alignment using Local All-Pass Filters

**Format :** Talk at Waseda University

**Author(s) :** Christopher Gilliam (University of Birmingham)

**Abstract :** The estimation of a geometric transformation that aligns two or more signals is a problem that has many applications. The problem occurs when signals are either recorded from two or more spatially separated sensors or when a single sensor is recording a time-varying scene, e.g., image registration, motion correction in medical imaging and time-varying delay estimation. In this talk we estimate the transformation by approximating it using a set of local all-pass (LAP) filters.

## [03596] Noise reduction in X-ray microspectroscopy

**Format :** Online Talk on Zoom

**Author(s) :** Jizhou Li (City University of Hong Kong)

**Abstract :** Investigating nanoscale morphological and chemical phase transformations is essential for a wide range of scientific and industrial applications across various disciplines. The emerging TXM-XANES imaging technique combines the strengths of full-field transmission X-ray microscopy (TXM) and X-ray absorption near edge structure (XANES) to generate chemical maps by capturing a series of multi-energy X-ray microscopy images and fitting them accordingly. However, its effectiveness is hindered by low signal-to-noise ratios due to system errors and insufficient exposure illuminations during rapid data acquisition. In this study, we present a straightforward and

robust denoising method that capitalizes on the inherent properties and subspace modeling of TXM-XANES imaging data to significantly improve image quality, paving the way for fast and highly sensitive chemical imaging. Comprehensive experiments using both synthetic and real datasets showcase the remarkable performance of our proposed approach.

## [03540] Remote Sensing Image Reconstruction from the Subspace Perspective

**Format :** Talk at Waseda University

**Author(s) :** Jie Lin (University of Electronic Science and Technology of China)

**Abstract :** Remote sensing images cover abundant spatial-spectral information while the images usually suffer from different degradations during the imaging and transmission. Image reconstruction is a fundamental step for subsequent applications. With improved imaging accuracy, the larger sizes of acquired images bring a greatly increased computation burden in reconstruction. In this talk, I will present matrix and tensor subspace-based methods for remote sensing image reconstruction, which enjoy satisfactory effects and lower computational complexity.

## [03879] Nonlocal Self-Similarity-Based Hyperspectral Remote Sensing Image Denoising With 3-D Convolutional Neural Network

**Format :** Talk at Waseda University

**Author(s) :** Zhicheng Wang (The University of Hong Kong)Michael Kwok-Po NG (The University of Hong Kong)Lina Zhuang (Key Laboratory of Computational Optical Imaging Technology, Aerospace Information Research Institute, Chinese Academy of Sciences, Beijing)Lianru Gao (Key Laboratory of Computational Optical Imaging Technology, Aerospace Information Research Institute, Chinese Academy of Sciences, Beijing)Bing Zhang (Aerospace Information Research Institute, Chinese Academy of Sciences, Beijing 100094, China, and also with the University of Chinese Academy of Sciences, Beijing)

**Abstract :** Deep-learning-based denoising methods for hyperspectral images have been comprehensively studied and achieved impressive performance. Compared with deep-learning-based methods, the nonlocal similarity-based methods are more suitable for images containing edges or regular textures. We propose a powerful denoising method, termed non-local 3-D convolutional neural network, combining traditional machine learning and deep learning techniques. The numerical and graphical denoising results of the simulated and real data show that the proposed method is superior to the state-of-the-art methods.

## [02628] Mathematical Modeling on waste reduction through sustainable developmnet.

**Session Time & Room :** 3D (Aug.23, 15:30-17:10) @D502

**Type :** Proposal of Minisymposium

**Abstract :** This study explores the use of sustainable inventory modeling as a tool for waste reduction in the context of manufacturing industries. Traditional inventory management models tend to prioritize cost reduction and efficiency, often leading to excess inventory and waste generation. The results suggest that sustainable inventory modeling can be a valuable approach for waste reduction and sustainability in manufacturing industries, providing a framework for organizations to achieve economic and environmental benefits while balancing the needs of various stakeholders.

**Organizer(s) :** Prof. Shiv Raj Singh, Dipti Singh.

**Classification :** 90-10, 90B05, 90B50, 90C31, 90C10, Mathematical Modeling, Inventory, Storage, reservoirs, Management decision making, Sensitivity, Integer Programming

**Minisymposium Program :** No registered information

# [02644] Black box methods for efficient learning in high-dimensional scientific computing

**Session Time & Room :** 1D (Aug.21, 15:30-17:10) @F310

**Type :** Proposal of Minisymposium

**Abstract :** The past decade has seen an explosion of interest in the use of black box modeling techniques in scientific computing. Driven by advances in hardware and software, researchers have begun to harness the power of these techniques to solve a wide range of complex and high-dimensional problems arising in computational science and engineering. This minisymposium aims to bring together experts from various fields including data science, high-dimensional approximation, deep learning, optimization, control, and scientific computing to share their latest research and developments in this exciting and rapidly evolving area of computational science.

**Organizer(s) :** Nick Dexter, Clayton Webster, Guannan Zhang

**Classification :** 41A46, 65D15, 65Y20, 94A20, 68T07

**Minisymposium Program :**

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02644 (1/1) : 1D @F310 [Chair: Nick Dexter]

## [05120] Is Monte Carlo a bad sampling strategy?

**Format :** Online Talk on Zoom

**Author(s) :** Ben Adcock (Simon Fraser University)Simone Brugiapaglia (Concordia University)

**Abstract :** When approximating smooth, high-dimensional functions from limited samples using polynomials, it is common to use Monte Carlo (MC) sampling to lessen the curse of dimensionality. However, it is well known that MC is theoretically suboptimal. This has led to a concerted effort to design improved strategies with near-optimal sample complexities. In this work we demonstrate, both theoretically and numerically, that MC is actually an eminently suitable strategy in sufficiently high dimension despite its apparent suboptimality.

## [05196] CAS4DL: Christoffel Adaptive Sampling for Deep Learning in data-scarce applications

**Format :** Online Talk on Zoom

**Author(s) :** Ben Adcock Juan M. Cardenas (Simon Fraser University)Nick Dexter (Florida State University)

**Abstract :** Many problems in computational science and engineering require the approximation of a high-dimensional function from data. In many such applications, data is costly to generate: for example, it each sample may require a costly PDE solve. Therefore, it is imperative to develop highly sample efficient algorithms. Recently, deep neural networks and deep learning have shown great promise to provide breakthrough performance in challenging function approximation tasks. In this work, we propose an adaptive sampling strategy, CAS4DL (Christoffel Adaptive Sampling for Deep Learning) to increase the sample efficiency of DL. Our novel approach is based on interpreting the second to last layer of a DNN as a dictionary of functions defined by the nodes on that layer. With this viewpoint, we then define an adaptive sampling strategy motivated by adaptive sampling schemes recently proposed for linear approximation schemes, wherein samples are drawn randomly with respect to the Christoffel function of the subspace spanned by this dictionary. We present numerical experiments comparing CAS4DL with standard Monte Carlo (MC) sampling. Our results demonstrate that CAS4DL often yields substantial savings in the number of samples required to achieve a given accuracy, particularly in the case of smooth activation functions. These results therefore are a promising step towards fully adapting DL towards scientific computing applications.

## [05283] Exploiting the local parabolic landscapes of adversarial losses to accelerate black-box adversarial attack

**Format :** Talk at Waseda University

**Author(s) :** Hoang Anh Tran (Oak Ridge National Laboratory)

**Abstract :** Machine learning models, and convolutional neural networks (CNNs) in particular, have demonstrated remarkable performance in many classification tasks. However, deep learning technology also exposed certain security risks, as they are susceptible to malicious inputs, which are small, human-imperceptible perturbations to

the inputs designed to fool the model prediction. In this talk, we present an investigation into the vulnerability of CNN classifiers from the shape of the loss's landscape perspective. We theoretically and experimentally justify that the adversarial losses of many standard and robust image classifiers behave like parabolas with respect to perturbations in the Fourier domain, but not in the pixel domain. Then, we exploit the parabolic landscape to design a new black-box adversarial attack methods with improved query efficiency, compared to the other state-of-the-art baselines. We demonstrate the efficiency of our method on MNIST, CIFAR-10 and ImageNet datasets for various standard and robust models.

## [05315] A Mathematical Approach Towards Physical Law Learning

**Format :** Online Talk on Zoom

**Author(s) :** Gitta Kutyniok (LMU Munich)Philipp Scholl (LMU Munich)Aras Bacho (LMU Munich)Holger Boche (TU Munich)

**Abstract :** For most of human history, scientists had to derive physical laws by hand. Recently, due to the data deluge, several learning-based approaches to infer the governing laws from experimental data have been suggested. However, a theoretical foundation is at present missing. In this talk, we will discuss our first stage of a mathematical framework for physical law learning, in particular, how to derive well-definedness of the learning problem, both theoretically and numerically.

## [02671] Recent advances on the analysis of hyperbolic balance laws

**Session Time & Room :**

02671 (1/2) : 5C (Aug.25, 13:20-15:00) @G605

02671 (2/2) : 5D (Aug.25, 15:30-17:10) @G605

**Type :** Proposal of Minisymposium

**Abstract :** Hyperbolic balance laws are of great interest owing to their importance in applications, such as the Euler equations, magnetohydrodynamic system, Boltzmann equations, and in applied mathematics. Recently, there have been a lot of advances in ascertaining the global well-posedness of such systems. The generic breakdown of classical solutions requires one to enlarge the space to hope for well-posedness or add 'good' source terms. The mathematical studies of these PDEs pose significant analytical/numerical challenges. This minisymposium seeks to bring together researchers to promote exchange of ideas, and present recent developments on the mathematical analysis and novel methods in this area.

**Organizer(s) :** Manas Bhatnagar, Geng Chen, Hailiang Liu

**Classification :** 35L40, 35L45, 35L65, 35L67

**Minisymposium Program :**

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02671 (1/2) : 5C @G605 [Chair: Manas Bhatnagar]

## [03611] Existence and Stability of Traveling Waves of Boussinesq-Burgers Equations

**Format :** Online Talk on Zoom

**Author(s) :** Kyle Kun Zhao (Tulane University)Anita Yang (Chinese University of Hong Kong)Zhian Wang (Hong Kong Polytechnic University)

**Abstract :** We introduce rigorous mathematical results concerning the existence and stability of traveling wave solutions to the Cauchy problem of the one-dimensional Boussinesq-Burgers equations modeling the propagation of weak tidal bores. Existence of traveling waves is obtained by means of phase plane analysis and geometric singular perturbation. Local stability of traveling waves with arbitrary strength is proven by spatially weighted energy methods.

## [04963] Global dynamics and photon loss in the Kompaneets equation

**Format :** Talk at Waseda University

**Author(s) :** Hailiang Liu (Iowa State University )

**Abstract :** The Kompaneets equation governs dynamics of the photon energy spectrum in certain high temperature (or low density) plasmas. We present several results concerning the long-time convergence of solutions to Bose-Einstein equilibria and the failure of photon conservation due to shock formation at the zero-energy boundary. This talk is based on a joint work with J. Ballew, G. Iyer, D. Levermore and R. Pego.

## [03629] HYPOCOERCIVITY OF STOCHASTIC GALERKIN FORMULATIONS FOR STABILIZATION OF KINETIC EQUATIONS

**Format :** Talk at Waseda University

**Author(s) :** Hui Yu (Tsinghua University)Stephan Gerster (Universit'a degli Studi dell'Insubria)Michael Herty (RWTH Aachen University)

**Abstract :** We consider the stabilization of linear kinetic equations with a random relaxation term. The well-known framework of hypocoercivity by J. Dolbeault, C. Mouhot and C. Schmeiser (2015) ensures the stability in the deterministic case. This framework, however, cannot be applied directly for arbitrarily small random relaxation parameters. Therefore, we introduce a Galerkin formulation, which reformulates the stochastic system as a sequence of deterministic ones. We prove for the gamma-distribution that the hypocoercivity framework ensures the stability of this series and hence the stochastic stability of the underlying random kinetic equation. The presented approach also yields a convergent numerical approximation.

## [04154] Traveling Wave Solutions in Keller-Segel Models of Chemotaxis

**Format :** Online Talk on Zoom

**Author(s) :** Tong Li (The University of Iowa)

**Abstract :** We study global existence and long-time behavior of solutions for hyperbolic-parabolic PDE models of chemotaxis.

We show the existence and the stability of traveling wave solutions to systems of nonlinear conservation laws derived from the Keller-Segel model. We construct biologically relevant oscillatory traveling wave solutions to an attractive chemotaxis system of mixed-type. Traveling wave solutions of chemotaxis models with growth are also investigated.

02671 (2/2) : 5D @G605 [Chair: Hailiang Liu]

## [04448] On the Riccati dynamics of 2D Euler-Poisson equations with attractive forcing

**Format :** Online Talk on Zoom

**Author(s) :** Yongki Lee (Georgia Southern University)

**Abstract :** The multi-dimensional Euler-Poisson system describes the dynamic behavior of many important physical flows. In this talk, a Riccati system that governs pressureless two-dimensional EP equations is discussed. The evolution of divergence is governed by the Riccati type equation with several nonlinear/nonlocal terms. Among these, the vorticity accelerates divergence while others further amplify the blow-up behavior of a flow. The growth of these blow-up amplifying terms are related to the Riesz transform of density, which lacks a uniform bound makes it difficult to study global solutions of the multi-dimensional EP system. We show that the Riccati system can afford to have global solutions, as long as the growth rate of blow-up amplifying terms is not higher than exponential, and admits global smooth solutions for a large set of initial configurations. Several recent works in a similar vein will be reviewed.

## [04918] Critical thresholds in spherically symmetric Euler-Poisson systems

**Format :** Talk at Waseda University

**Author(s) :** Manas Bhatnagar (University of Massachusetts Amherst)

**Abstract :** We will see an introduction to the concept of Critical Threshold Phenomena (CTP) and how it plays a role in the Euler-Poisson systems. We will go over some of the existing results in this area and how the techniques have developed over time. In the end, we will see some new results on the multidimensional spherically symmetric Euler-Poisson systems.

## [04518] On multi-dimensional rarefaction waves

**Format :** Talk at Waseda University

**Author(s) :** Tianwen Luo (Tsinghua University)Pin Yu (Tsinghua University)

**Abstract :** We study the two-dimensional acoustical rarefaction waves under the irrotational assumptions. We provide a new energy estimates without loss of derivatives. We also give a detailed geometric description of the rarefaction wave fronts. As an application, we show that the Riemann problem is structurally stable in the regime of two families of rarefaction waves. This is a joint work with Prof. Pin Yu in Tsinghua University.

## [04947] Nonlocal traffic flow models

**Format :** Talk at Waseda University

**Author(s) :** Thomas Hamori (University of South Carolina)Yongki Lee (Georgia Southern University)Yi Sun (University of South Carolina)Changhui Tan (University of South Carolina)

**Abstract :** In this talk, I will discuss a family of traffic flow models. The conventional Lighthill-Whitham-Richards model is notorious for exhibiting finite-time shock formation for all generic initial data. To address this issue, I will introduce a family of nonlocal traffic flow models, which incorporate look-ahead interactions. These models can be derived from discrete cellular automata models. Interestingly, we will explore how the nonlocal slowdown interactions prevent the shock formation, under certain suitable settings. Furthermore, I will also discuss the extension of these nonlocal models to second-order traffic flow models.

# [02700] Recent developments on Infinite Dimensional Analysis, Stochastic Analysis and Quantum Probability

**Session Time & Room :**

02700 (1/2) : 1C (Aug.21, 13:20-15:00) @E501

02700 (2/2) : 1D (Aug.21, 15:30-17:10) @E501

**Type :** Proposal of Minisymposium

**Abstract :** There has been a great achievement of the theory in both white noise analysis (as an infinite dimensional analysis) and quantum probability theory starting from the seventies of the last century. These two theories have been developed and unified in order to get important directions on the quantum information theory, quantum computation and etc. In this session we would like to discuss connections between white noise analysis and quantum information theory through the experts' talks in each fields including the mathematical finance.

**Organizer(s) :** Isamu Dokur, Kimiaki Saito

**Classification :** 60H40, 81P45, 60H30, 46L53, 68Q11, White Noise Theory, Quantum Information, Applications of stochastic analysis, Noncommutative probability and statistics, Information complexity

**Minisymposium Program :**

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02700 (1/2) : 1C @E501 [Chair: Kimiaki Saito, Isamu Dokur]

## [02940] Note on complexities for the quantum compound systems

**Format :** Talk at Waseda University

**Author(s) :** Noboru Watanabe (Tokyo University of Science)

**Abstract :** In order to discuss the efficiency of information transmission of the quantum communication processes consistently, we consider the entropy type functional and the mutual entropy type functional with respect to the initial state and the quantum communication channel. In this study, the mutual entropy type measures are constructed by the compound states between the initial and final systems.

We modify the compound states and examine the entropy functional and the mutual entropy functional defined by the modified compound states by means of the initial state and the completely positive channel to study the efficiency of information transmission of the quantum communication processes.

## [03589] Asymptotics of densities of first passage times for spectrally negative Lévy processes

**Format :** Talk at Waseda University

**Author(s) :** shunsuke kaji (meijo university)

**Abstract :** We study a first passage time of a Lévy process over a positive constant level. In the spectrally negative case we give conditions for absolutely continuity of the distributions of the first passage times. The tail asymptotics of their densities are also clarified, where the asymptotics depend on tail behaviour of the corresponding Lévy measures.

## [03953] A combinatorial formula of the moments of a deformed filed operator

**Format :** Talk at Waseda University

**Author(s) :** Nobuhiro ASAI (Aichi University of Education)

**Abstract :** We shall construct the two parameterized deformed Fock space obtained from the weighted  $q$ -deformation technique. We shall explain a combinatorial moment formula of a Poisson type filed operator defined on this Fock space by using the set partitions with their statistics. In addition, we shall mention relationships with the recurrence formula for the orthogonal polynomials of the deformed Poisson distribution. This talk is based on the joint work with H. Yoshida (Ochanomizu Univ, Tokyo).

02700 (2/2) : 1D @E501 [Chair: Kimiaki Saito]

## [02981] Multiplication Operators by White Noise Delta Functions and Associated Differential Equations

**Format :** Talk at Waseda University

**Author(s) :** Un Cig Ji (Chungbuk National University)

**Abstract :** We establish explicit forms of the multiplication operators induced by white noise delta functions, which are closely related to the Bogoliubov transformation and a quantum analogue of Girsanov transform. Then we study the differential equations for operators associated with the multiplication operators by the white noise delta functions. This talk is based on a joint work with L. Accardi and K. Saito.

## [03986] Positivity of Q-matrices and quadratic embedding constants of graphs

**Format :** Talk at Waseda University

**Author(s) :** Nobuaki Obata (Tohoku University)

**Abstract :** Let  $G = (V, E)$  be a graph. Positivity of the Q-matrix  $Q = Q_q = [q^{d(x,y)}]$  is essential for q-deformed vacuum state of a graph and q-deformed CLT for a growing graph. Positivity of  $Q_q$  is profoundly related to conditional negativity of the distance matrix  $D = [d(x,y)]$ . It is shown that the positivity region of  $Q_q$  contains \$

**[0,1] if and only if the quadratic embedding constant (QEC) of  $G$  is non-positive. We report some results in this line and discuss open questions.**

## [03056] Data-driven methods to discover within-host biological dynamics

**Session Time & Room :** 5D (Aug.25, 15:30-17:10) @E804

**Type :** Proposal of Minisymposium

**Abstract :** Our minisymposium brings together researchers whose goal is to develop and apply algorithms towards discovering and documenting within-host dynamics of the immune system and infectious disease. One of the common challenges of this field is the degree to which existing databases of prior knowledge should be incorporated to enhance the analysis of new bioinformatic data sets. Presenters will discuss their varied research projects in this space. Throughout the minisymposium, we aim to foster a dialogue among the presenters, as well as minisymposium participants, from which the nuances of this field can be discussed.

**Organizer(s) :** Manuchehr Aminian, Michael Kirby

**Classification :** 68T09, 62P10, 92C42, 68T50

**Minisymposium Program :**

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03056 (1/1) : 5D @E804 [Chair: Manuchehr Aminian]

## [03279] How to find a pertinent research question: the identification and exploration of known unknowns

**Format :** Online Talk on Zoom

**Author(s) :** Mayla R Boguslav (Colorado State University)Nourah M Salem (University of Colorado Anschutz Medical Campus)Elizabeth White (University of Colorado Anschutz Medical Campus)Katherine J Sullivan (University of Colorado Anschutz Medical Campus)Michael Bada (University of Colorado Anschutz Medical Campus)Teri L Hernandez (University of Colorado Anschutz Medical Campus)Sonia M Leach (National Jewish Health)Lawrence E Hunter (University of Colorado Anschutz Medical Campus)Michael Kirby (Colorado State University)

**Abstract :** Scientific discovery progresses by exploring new and uncharted territory. More specifically, it advances by a process of transforming unknown unknowns first into known unknowns, and then into knowns. Over the last few decades, researchers have developed many knowledge bases to capture and connect the knowns, which has enabled topic exploration and contextualization of experimental results. But recognizing the unknowns is also critical for finding the most pertinent questions and their answers. Little work has focused on how scientists might use them to trace a given topic or experimental result in search of open questions and new avenues for exploration. We present methods and tools to help researchers automatically uncover these unknowns through the illumination of specific goals for scientific knowledge.

## [05174] A summary of algorithms for sparse feature selection for Biological Data

**Format :** Online Talk on Zoom

**Author(s) :** Michael Kirby (Colorado State University)

**Abstract :** Biological data sets such as transcriptomics, proteomics or metabolomics are characterised by their high dimension n and small sample size p. Realistically, it is a daunting challenge to deduce meaningful biological mechanisms when  $p <$

## [03409] Improving decoy detection for protein-protein interaction models

**Format :** Online Talk on Zoom

**Author(s) :** Corey OHern (Yale University)

**Abstract :** Computational prediction and design of proteins is a difficult task that results in models with a wide variation in quality. Decoy detection algorithms seek to classify computational models as high-quality or low-quality without knowledge of the experimental structures. Recently, dramatic improvements have been made in decoy detection of models for single proteins, but decoy detection of protein-protein interface (PPI) models is still challenging. To assess the current state-of-the-art for PPI decoy detection, we scored computational models generated using rigid-body docking software, ZDOCK, from a dataset of 33 heterodimeric high-resolution x-ray crystal structures against a standard measure of similarity to the x-ray crystal structures. We found that for some targets there is a strong correlation between the docking and ground truth scores (i.e. easy targets), whereas for other targets there are only weak correlations (i.e. difficult targets). We show that a metric that characterizes the “flatness” of the target interfaces can distinguish easy from difficult targets, where flat targets possess only weak correlations between the docking and ground truth scores. In addition, most rigid docking software methods generate highly imbalanced datasets containing mostly low-quality computational models. Balanced datasets of PPI models reduce sampling bias, which makes it easier to identify the physical features that can classify PPI computational models.

## [05206] Early Detection of Disease: An intersection between artificial intelligence and biomathematics

**Format :** Online Talk on Zoom

**Author(s) :** Juan B Gutierrez (University of Texas at San Antonio)

**Abstract :** Many states of disease are progressive, having a silent phase in which pathogenesis advances without the manifestation of any symptoms. However, small perturbations can be detected by a complex signal such as electrocardiography. In this talk, I will present how to approach the detection of subtle physiological signals through the systematic design of the architecture of an artificial neural network capable of detecting liver-stage malaria with an accuracy of +90%.