MONASH University

The 22nd Biennial Computational Techniques and Applications Conference

Monash University, Melbourne, Australia

19–22 November, 2024

Updated: November 19, 2024. Editors: Ricardo Ruiz Baier, Jai Tushar.

Acknowledgement of Traditional Owners

Monash University acknowledges that its Australian campuses are located on the unceded lands of the people of the Kulin Nations, and pay our respects to their Elders, past and present. We acknowledge that Australia's Indigenous peoples were this country's first scientists, and we thank their connection to country and their knowledge which continues to shape our work today.

Support

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School of Mathematics, Monash University

Australian Mathematical Sciences Institute

Mathematics of Computation and Optimisation (MoCaO) special interest group of AustMS

Society for Industrial and Applied Mathematics (SIAM)

The ANZIAM Student Support Scheme

Plenary and public lecture speakers

- Santiago Badia, Monash University, Australia
- Fleurianne Bertrand, Technische Universität Chemnitz, Germany
- Victor Calo, Curtin University, Australia
- Carsten Carstensen, Humboldt-Universität zu Berlin, Germany
- Vivien Challis, Queensland University of Technology, Australia
- Nilima Nigam, Simon Fraser University, Canada
- Terence O'Kane, Commonwealth Scientific and Industrial Research Organisation, Australia
- Vijay Rajagopal, University of Melbourne, Australia
- Dingxuan Zhou, University of Sydney, Australia

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Program compilation

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Welcome

The 22nd Biennial Computational Techniques and Applications Conference (CTAC2024) is hosted by the School of Mathematics at Monash University, Melbourne.

CTAC is organised by the special interest group in computational techniques and applications of ANZIAM, the Australian and New Zealand Industrial and Applied Mathematics Division of the Australian Mathematical Society. The meeting will provide an interactive forum for researchers interested in the development and use of computational methods applied to engineering, scientific and other problems. The CTAC meetings have been taking place biennially since 1981, the most recent being held in 2022 at QUT.

A refereed proceedings will be published after the conference in the Electronic Supplement of the ANZIAM Journal. This will be subject to the usual rigorous ANZIAM J. refereeing process.

This year we have two student prizes, one sponsored by MoCaO and the other by AMSI. Student talks are denoted in the conference program and list of abstracts by an asterisk. The student prize committee is led by Janosch Rieger and Antoine Marteau.

We hope you enjoy the conference.

Information

Conference venue

The conference is hosted at Monash University, Clayton Campus.

All plenary, public, and contributed talks on Tuesday 19 November (as well as registration and afternoon tea) will be in the Eastern Science Lecture Theatres S1-S4. On Wednesday-Thursday-Friday, all talks as well as morning and afternoon teas, will be at the Woodside Building for Technology and Design, a short distance from the Science Lecture theatres and Monash Club. Plenary talks are in the lower level (room LG02) while the contributed talks will be in rooms G06, G15 (ground level) and 1.04, 1.06 (first floor).

The Computational Mathematics Group meeting will be held in room LG02 of the Woodside building.

Presentations

All plenary talks are around 50 minutes long, followed by 10 minutes of Q&A time.

All contributed talks are 20 minutes long, plus 5 minutes for questions, discussion and changeover. The session chair will give you a signal when you have spoken for 18 minutes. Please do not exceed your time. Each room is equipped with a projector and screen, and a desktop computer running Windows, with usual PowerPoint, PDF and web browsers. Please ensure your presentation is in one of these formats. Connecting your own laptop is possible, but this is only recommended if you really require it (e.g., if your presentation is not one of the formats above), and you are responsible for arranging this with the session chair ahead of time.

Internet access

Monash offers Free Guest Public Wifi to guests and visitors to its campuses. Alternatively, you may use your home institution's login with Eduroam.

Social events

The welcome reception with drinks and canapés will be held at Monash Club on Tuesday 19 November, 18:30-20:30.

The conference dinner will be held at The Sandringham Yacht Club on Thursday 21 November, 18:30-22:00. CTAC will provide shuttle transportation for all participants, which will be available at 17:40 on the parking right outside of the Woodside building (link to map).

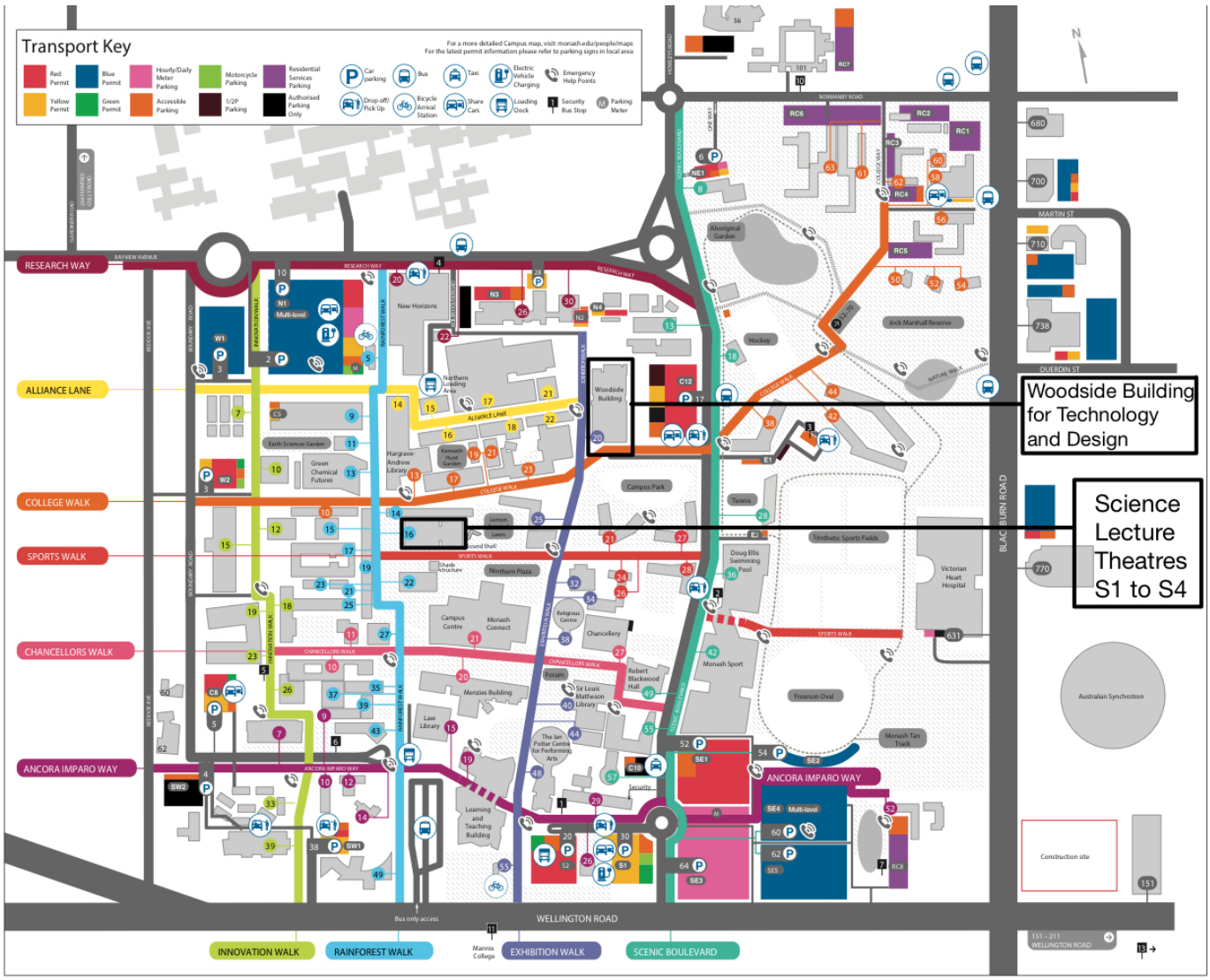
Dining

Morning and afternoon teas will be provided by CTAC. For lunch you can find a number of nice places in campus. A guide can be found in this link.

Coffee in Melbourne is excellent. In campus we can recommend The Church of Secular Coffee and Cafelito.

Other activities

While in Melbourne, you can try the Summer Night Market at the historic Queen Victoria Market, starting on Wednesday November 20th, or go to Westerfolds Park around sunset to see the wildlife.


Transport Key
RESEARCH WAY
ALLIANCE LANE
COLLEGE WALK
SPORTS WALK
CHANCELLORS WALK
ANCORA IMPARO WAY
WELLINGTON ROAD
INNOVATION WALK
RAINFOREST WALK
EXHIBITION WALK
SCENIC BOULEVARD
Woodside Building for Technology and Design
Science Lecture Theatres S1 to S4

Campus map

Programme

Tuesday 19 November

10:00-11:35 **Registration in the Science Auditorium S1-S4 foyer**

11:35-12:00 **Science Auditorium S4**

Introductory remarks (Ricardo Ruiz Baier)
Welcome address (Jordan Nash - Dean, Faculty of Science)
Survey (Adriana Zanca)

Plenary talk Chair: Bishnu Lamichhane

12:00-13:00 Nilima Nigam (p.18)
Skeletal muscles: modeling and simulation

13:00-14:15 **Lunch break**

	S1 Chairs: Jérôme Droniou	S2 Ricardo Oyarzúa	S3 Adriano Festa	S4 Tim Moroney
14:15-14:40	Daniele Boffi (p.34) *On a virtual element method for the acoustic eigenvalue problem*	Lucia Gastaldi (p.50) *A fictitious domain approach for the finite element discretization of FSI*	Felipe Atenas (p.60) *First-order proximal splitting methods for distributed optimization*	Alexander Gilbert (p.22) *A complex-projected Rayleigh quotient iteration for targeting interior eigenvalues*
14:40-15:05	Andrea Borio (p.34) *Stabilization-Free VEM Part I: primal and mixed lowest order methods*	Tamara Tambyah* (p.58) *Space–time energy and entropy conservation for the thermal shallow water equations*	Kaniz Fatema* (p.61) *A new local search algorithm for solving constrained DC optimisation*	Verónica Anaya (p.21) *Finite element approximation for the unsteady Brinkman – Forchheimer equations*
15:05-15:30	Stefano Berrone (p.33) *Stabilization-Free VEM Part II: Construction details and higher-order schemes*	Miguel Serón* (p.57) *A residual-based a posteriori error estimator for a non-isothermal Navier-Stokes/Darcy coupled system*	Yiming Ying (p.64) *Interplay between machine learning and optimisation*	Leonardo A. Poveda (p.26) *An exponential integration constraint energy minimizing generalized multiscale method for parabolic problems*

15:30-16:05	**Afternoon tea**			
	S1 Chairs: Jai Tushar	S2 Segundo Villa Fuentes	S3 Yiming Ying	S4 Ricardo Ruiz Baier
16:05- 16:30	Jörn Wichmann (p.68) *Reaching the equilibrium: Long-term stable numerical schemes for SPDEs*	Riski Kurniawan* (p.52) *Smoothed particle hydrodynamics for simulating heat transfer with mixed boundary conditions*	Elizabeth Harris* (p.62) *Calculating minimum volume covering ellipsoids using leverage score sampling*	Agus Soenjaya* (p.27) *Finite element method for a micromagnetic model at elevated temperatures*
16:30- 16:55	Kaustav Das (p.65) *On stochastic PDEs and their applications to derivative pricing through a conditional Feynman-Kac formula*	Anne Boschman (p.49) *Phase-field modelling of adhesive interfaces*	Duong Ton Thai Duong (p.61) *New similarity-distance technique of intutionistic Fuzzy sets*	Riley Whebell (p.28) *Towards a multi-scale model of sugarcane bagasse chemical pre-treatment using microCT imaging*
Public lecture	Chair: Mark Flegg			
17:00-18:00	Terence O'Kane (p.19) *Mathematical methods and artificial intelligence in climate science*			
18:00 18:15	Survey information			
18:30-20:30	**Monash Club** **Drinks reception**			

Wednesday 20 November

Plenary talk — Chair: Ian Sloan

9:00-10:00 — Dingxuan Zhou (p.19)
Mathematical theory of structured deep neural networks

10:00-10:35 Morning tea

	G06 Chairs: Jai Tushar	G15 Ricardo Oyarzúa	1.04 Matthew Tam	1.05 Verónica Anaya
10:35-11:00	David Mora (p.37) *Stream virtual element methods for the Navier-Stokes equations with pressure recovery*	Connor Mallon* (p.53) *Adsorption system topology optimisation*	Janosch Rieger (p.62) *Generalised Gearhart-Koshy acceleration is a Krylov space method*	Josiah Murray* (p.25) *Numerical inversion of the Laplace transform with application to modelling railway transition zones*
11:00-11:25	Andres E. Rubiano* (p.38) *A posteriori error analysis of robust virtual element methods for stress-assisted diffusion problems*	Luis F. Gatica (p.50) *A posteriori error analysis of a mixed FEM for the stationary convective Brinkman–Forchheimer problem*	Linda Stals (p.63) *Faut tolerant multigrid*	Rudi A. Prihandoko* (p.26) *Stable dual pairing summation-by-parts operator for sediment transport model with well-posed boundary conditions*
11:25-11:50	Ayush Agrawal* (p.33) *Analysis of LDG method for non-linear fractional Rayleigh–Stokes problem with variable coefficient on the non-uniform mesh*	Jingyu Liu* (p.53) *Analysis of the staggered DG method for the quasi-Newtonian Stokes flows*	Xiyue Guan* (p.62) *Mixed precision in hierarchical basis finite element methods*	Tau Keong Ang (p.23) *The impacts of mortality rate and strong Allee effect in a three-species food chain model with Crowley-Martin functional response*

Plenary talk — Chair: Jérôme Droniou

11:50-12:50 — Carsten Carstensen (p.17)
Lower eigenvalue bounds for the harmonic and bi-harmonic operator

12:50-13:00 Group photo

13:00-14:15 Lunch break

	G06 Chairs: David Mora	G15 Lucia Gastaldi	1.04 Linda Stals	1.05 Jennifer Flegg
14:15- 14:40	Jai Tushar (p.38) *A discrete trace theory for non-conforming polytopal hybrid discretisation methods*	Huateng Zhu* (p.59) *Convergence analysis of numerical approximations for total variation flow*	Matthew K. Tam (p.63) *A decentralised algorithm for min-max problems*	Jordan Shaw-Carmody* (p.27) *Optimising mesh refinement for the reaction-diffusion-convection equation using AFEM*
14:40- 15:05	Rekha Khot (p.36) *Hybrid high-order methods for the wave equation in first-order form*	Kieran Ricardo (p.56) *Thermodynamic consistency and structure-preservation in summation by parts methods for the moist compressible Euler equations*	Adriano Festa (p.61) *A network model for urban planning based on a coupling between a Mean-Field Game and an optimal transportation problem*	Shahak Kuba* (p.24) *Using ODEs to solve an evolving interface problem*
15:05- 15:30	Marwa Salah* (p.38) *Serendipity discrete complexes with enhanced regularity*	Isaac Bermúdez* (p.49) *A conforming mixed finite element method for a coupled Navier–Stokes and transport system modelling reverse osmosis*	Zachary J. Wegert* (p.64) *Parallel level set-based optimisation of three-dimensional piezoelectric materials*	Domenic Germano (p.30) *Jump-Switch-Flow: hybrid deterministic-stochastic trajectories of compartmental systems*
15:30- 15:55	Weifeng Qiu (p.37) *A C0 interior penalty method for mth-Laplace equation*	Bishnu Lamichhane (p.52) *A mixed finite element method for extended Fisher-Kolmogorov equation based on biorthogonal systems*	~~Liam Timms~~* (p.63) ~~*Coordinating a virtual power plant with a decentralised distributed algorithm*~~	Sadia Arshad (p.29) *Numerical framework for a dengue model governed by fractional derivative with singular and non-singular kernels*
15:55-16:30	**Afternoon tea**			
Plenary talk	Chair: Jennifer Flegg			
16:30-17:30	Vijay Rajagopal (p.19) *What do we need in a computational physiology framework to predict single cell biology?*			

Thursday 21 November

Plenary talk — Chair: Lucia Gastaldi

09:00-10:00 — Victor Calo (p.16)
Adaptive stabilized finite element methods: A variational multiscale approach for robust and accurate flow simulations

10:00-10:35 Morning tea

	G06 Chairs: Daniele Boffi	G15 Segundo Villa Fuentes	1.04 Sergio Rojas	1.05 Anne Boschman
10:35- 11:00	Jérôme Droniou (p.35) *Design and analysis of an extended virtual element method*	Noura Alhawiti* (p.48) *A mixed FEM for curve diffusion flow problem in one dimension using bi-orthogonal systems*	Alexandre Magueresse* (p.44) *Energy minimisation using tensor-product free-knot B-splines*	Mark B. Flegg (p.30) *Developments in stochastic reaction-diffusion algorithms*
11:00- 11:25	Raman Kumar (p.36) *Hybrid high-order methods for extended Fisher-Kolmogorov and Fisher-Kolmogorov equation*	Harvindra Singh* (p.57) *An efficient pseudospectral approximation of non-Linear time-evolution equations*	Terence O'Kane (p.45) *Bayesian structure learning for climate model evaluation*	Bruce Ruishu Jin (p.31) *Block structured adaptive mesh refinement immersed boundary-lattice Boltzmann method and applications in flapping-wing and engineering flows*
11:25- 11:50	Jia Jia Qian* (p.37) *A discrete de Rham method for Einstein's equations*	Thien Phan (p.55) *A DEM numerical framework to model jamming gripper*	Gaurav Gupta (p.42) *Leveraging machine learning for macroeconomic forecasting*	Mark George* (p.22) *Mass-conserving immersed boundary method for coupled incompressible solvers on collocated finite volume grids*

Plenary talk — Chair: Eun-Jae Park

11:50-12:50 — Fleurianne Bertrand (p.15)
Stress-based finite elements methods

12:50-14:15 Lunch break

	G06 Chairs: Jörn Wichmann	G15 Bishnu Lamichhane	1.04 Janosch Rieger	1.05 Mark Flegg
14:15- 14:40	Quoc Thong Le Gia (p.67) *Bayesian inference calibration of the modulus of elasticity*	Jordi Manyer* (p.54) *Scalable solvers for the inductionless Magneto-Hydrodynamics (MHD) equations at high Hartmann numbers*	Stefano Berrone (p.40) *A posteriori error estimates and adaptive mesh refinement for variational physics informed neural networks*	Tim Moroney (p.24) *A spectral method for two-dimensional partial differential equations on irregular domains*
14:40- 15:05	Peter Kritzer (p.67) *Function space embeddings and L_∞-approximation with infinitely many variables*	Antoine Marteau (p.54) *Multiscale models for nonlinear transient electromagnetic problems with confined eddy currents*	Sergio Rojas (p.46) *Robust variational physics-informed neural networks*	Matthew Fernandes* (p.66) *An efficient surrogate model for inversion of a class of wave configuration parameter*
15:05- 15:30	Sang-Hyeok Lee (p.67) *Forecasting shipping freight rates and PDEs for their derivatives*	Ricardo Oyarzúa (p.55) *Analysis of a FEM with exactly divergence-free magnetic field for the stationary MHD problem*	Wei Li* (p.44) *Compatible finite element interpolated neural networks*	Sharen J. Cummins (p.21) *Modelling coupled particle/air flow in industrial turbomachinery devices using a ghost cell immersed boundary method*
15:30- 15:55	Ian H. Sloan (p.68) *Doubling the convergence rate with kernel approximation*	Aamir Yousuf* (p.59) *Numerical analysis of a coupled thermoelastic–diffusion plate model*	Ati Rostami* (p.46) *Improving Thornley's Model and Investigating Identifiability of its Parameters*	Dougal Stewart* (p.28) *A dual pairing summation-by-parts finite difference framework for nonlinear conservation laws*
15:55-16:30	**Afternoon tea**			
16:30-17:40	**CMG Meeting** (Chair: Linda Stals)			
17:40-18:30	**Bus ride to Sandringham**			
18:30-22:00	**Conference Dinner**			

Friday 22 November

Plenary talk — Chair: Tim Moroney

09:00-10:00 — Vivien Challis (p.18)
Computational structural optimisation of piezoelectric materials

10:00-10:35 Morning tea

	G06 Chairs: Rekha Khot	G15 Ricardo Oyarzúa	1.04 Terence O'Kane	1.05 Alexander Gilbert
10:35-11:00	Eun-Jae Park (p.37) *Some new staggered DG methods on polygonal meshes*	Arbaz Khan (p.51) *Recent advances in numerical approximations for optimal control of fluid flow problems*	Subhashis Chatterjee (p.41) *Adaptive fuzzy inference system-based deep learning model for software dependability analysis*	Puneet Rana (p.27) *Linear and weakly nonlinear stability analyses in Horton-Rogers-Lapwood non-Newtonian nanofluid model*
11:00-11:25	Ruchi Guo (p.35) *How flexible are the element shapes for VEM?*	David Lee (p.52) *Helmholtz preconditioning for multi-scale atmospheric dynamics*	Vinesha Peiris (p.45) *Kolmogorov-Arnold theorem and its applications*	Stuart Hawkins (p.23) *A fast high order algorithm for multiple scattering from large configurations of scatterers*
11:25-11:50	Santimoy Kundu (p.51) *Case wise study of surface waves in a hydrostatic stress magneto-elasticity composite model*	Segundo Villa Fuentes (p.58) *New twofold saddle-point formulations for poroelasticity with porosity-dependent permeability*	Difeng Cai (p.40) *Universal monotonic flow-based generative models via latent dynamics*	Ravindra Pethiyagoda (p.25) *Compressible ocean waves generated by sudden seabed rise near a step-type topography*
11:50-12:15	Mi-Young Kim (p.36) *DG-DGLM method and linear solver for hyperbolic conservation laws*	Cristian Carcamo (p.49) *Frequency-domain formulation and convergence analysis of Biot's poroelasticity equations based on total pressure*	Vassili Kitsios (p.43) *Climate reduce-order modelling: Galerkin projection of the atmospheric equations of motion onto an orthogonal basis*	Erik Garcia Neefjes (p.66) *A neural-network surrogate Bayesian algorithm for the Helmholtz inverse-shape problem*

Plenary talk — Chair: Ricardo Ruiz Baier

12:15-13:15 — Santiago Badia (p.14)
Finite element interpolated neural networks

13:15-13:30 Closing and proceedings information

Plenary talks

Public lecture

* * *

Finite element interpolated neural networks

Santiago Badia (Monash University)

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We propose a general framework for solving forward and inverse problems constrained by partial differential equations, where we interpolate neural networks onto adaptive finite element spaces to represent the (partial) unknowns. The framework overcomes the challenges related to the imposition of boundary conditions, the choice of collocation points in physics-informed neural networks, and the integration of variational physics-informed neural networks. A numerical experiment set confirms the framework capability of handling various forward and inverse problems. In particular, the trained neural network generalises well for smooth problems, beating finite element solutions by some orders of magnitude in some cases. We propose an effective one-loop solver with an initial data fitting step (to obtain a cheap initialisation) to solve inverse problems. We consider problems posed in H(div) and H(curl), as well as the combination of the proposed technology with unfitted finite element methods.

Stress-based finite elements methods

Fleurianne Bertrand (Technische Universität Chemnitz, Germany)

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This talk explores recent advancements in stress and flux-based finite element methods. It focuses on addressing the limitations of traditional finite elements, in order to describe complex material behavior and engineer new metamaterials. Stress and flux-based finite element methods are particularly useful in error estimation, laying the groundwork for adaptive refinement strategies. This concept builds upon the hypercircle theorem which states that in a specific energy space, both the exact solution and any admissible stress field lie on a hypercircle. However, the construction of finite element spaces that satisfy admissible states for complex material behavior is not straightforward. It often requires a relaxation of specific properties, especially when dealing with non-symmetric stress tensors [2] or hyperelastic materials. Alternatively, methods that directly approximate stresses can be employed, offering high accuracy of the stress fields and adherence to physical conservation laws. However, when approximating eigenvalues, this significant benefit for the solution's accuracy implies that the solution operator cannot be compact. To address this, the solution operator must be confined to a subset of the solution that excludes the stresses. Yet, due to compatibility conditions, the trial space for the other solution components typically does not yield the desired accuracy. The second part of this talk will therefore explore the Least-Squares method as a remedy to these challenges [2,3]. To conclude this talk, we will emphasize the integration of those methods within global solution strategies, with a particular focus on the challenges regarding model order reduction methods [4].

[1] F. Bertrand, B. Kober , M. Moldenhauer, and G. Starke. Weakly symmetric stress equilibration and a posteriori error estimation for linear elasticity. Numerical Methods for Partial Differential Equations 37(4), 2021.

[2] F. Bertrand, and D. Boffi. First order least-squares formulations for eigenvalue problems. IMA Journal of Numerical Analysis 42.2 1339-1363, 2022.

[3] F. Bertrand, and D. Boffi. Least-squares formulations for eigenvalue problems associated with linear elasticity. Computers & Mathematics with Applications 95 19-27, 2021.

[4] F. Bertrand, D. Boffi and A. Halim. A reduced order model for the finite element approximation of eigenvalue problems. Computer Methods in Applied Mechanics and Engineering 404, 2023.

Adaptive stabilized finite element methods: A variational multiscale approach for robust and accurate flow simulations

Victor Calo (Curtin University)

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We present an Adaptive Stabilized Finite Element Method (AS-FEM) for tackling complex advection–diffusion–reaction equations and incompressible Stokes flows, employing residual minimization onto dual discontinuous-Galerkin norms. Our method is reinterpreted through a variational multiscale framework, where we decompose the solution into coarse and fine scales, enabling robust adaptivity and accurate error estimation. By formulating the problem as a saddle-point system, AS-FEM achieves a stable, continuous solution while delivering an on-the-fly error estimator that drives automatic mesh refinement. This ensures computational efficiency and solution accuracy even in heterogeneous, anisotropic, and advection-dominated cases.

Our approach extends to linear and nonlinear problems, including time-dependent scenarios, achieving reliable performance and optimal convergence rates. The method's flexibility and precision are demonstrated in applications like the Bratu equation, Laplace eigenvalue problem, and convection-dominated flows, where we achieve significant stability and fidelity in solution quality. Combining stability, adaptivity, and multiscale decomposition, this framework offers a powerful tool for advancing computational fluid dynamics and complex engineering simulations

Lower eigenvalue bounds for the harmonic and bi-harmonic operator

Carsten Carstensen **(**Humboldt-Universität zu Berlin, Germany)

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Collaborators: Sophie Puttkammer (Berlin), Ngoc Tien Tran (Augsburg), and Benedikt Gräßle (Berlin)

Recent advances in the nonconforming FEM approximation of elliptic PDE eigenvalue problems include the guaranteed lower eigenvalue bounds (GLB) and its adaptive finite element computation. Like guaranteed upper eigenvalue bounds with conforming finite element methods, GLB arise naturally from the min-max principle, also named after Courant, Fischer, Weyl. The first part introduces the derivation of GLB for the simplest second-order and fourth-order eigenvalue problems with relevant applications, e.g., for the localization of in the critical load in the buckling analysis of the Kirchhoff plates. The second part studies an optimal adaptive mesh-refining algorithm for the effective eigenvalue computation for the Laplace and bi-Laplace operator with optimal convergence rates in terms of the number of degrees of freedom relative to the concept of nonlinear approximation classes. The third part presents a modified hybrid high-order (HHO) eigensolver in the spirit of Carstensen, Ern, and Puttkammer [Numer. Math. 149, 2021] that directly computes guaranteed lower eigenvalue bounds under the idealized hypothesis of exact solve of the generalized algebraic eigenvalue problem and a mild explicit condition on the maximal mesh-size in a simplicial mesh. The error analysis allows for a priori quasi-best approximation and L2 error estimates as well as a stabilization-free reliable and efficient a posteriori error control. The associated adaptive mesh-refining algorithm performs well in computer benchmarks with striking numerical evidence for optimal higher convergence rates.

[1] C. Carstensen, A. Ern, and S. Puttkammer, Guaranteed lower bounds on eigenvalues of elliptic operators with a hybrid high-order method, Numer. Math. 149 (2021), 273–304.

[2] C. Carstensen and D. Gallistl, Guaranteed lower eigenvalue bounds for the biharmonic equation, Numer. Math. 126 (2014), 33–51.

[3] C. Carstensen and J. Gedicke, Guaranteed lower bounds for eigenvalues, Math. Comp. 83 (2014), 2605–2629.

[4] C. Carstensen, B. Gräßle, and N. T. Tran, Adaptive hybrid high-order method for guaranteed lower eigenvalue bounds. Numer. Math., volume 156, pp. 813–851, 2024.

[5] C. Carstensen and S. Puttkammer, Direct guaranteed lower eigenvalue bounds with optimal a priori convergence rates for the bi-Laplacian, SIAM J. Numer. Anal., volume 61, pp. 812–836, 2023.

[6] C. Carstensen and S.Puttkammer, Adaptive guaranteed lower eigenvalue bounds with optimal convergence rates, Numer. Math., volume 156, pp. 1–38, 2024.

[7] C. Carstensen, Q. Zhai, and R. Zhang, A skeletal finite element method can compute lower eigenvalue bounds, SIAM J. Numer. Anal. 58 (2020), 109–124.

Computational structural optimisation of piezoelectric materials

Vivien Challis (Queensland University of Technology)

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Structural optimisation is a powerful computational approach for designing structures or microstructures for particular physical properties. The approach combines numerical solution of the relevant state equations with a density- or level set-based description of the structure that facilitates optimisation of the design objective. I'll introduce structural optimisation and outline the common approaches. I'll then introduce the phenomenon of piezoelectricity and present details of our recent work optimising new periodic microstructures for both stiffness and piezoelectric response. Such microstructures are manufacturable by exploiting modern 3D printing technologies and I'll talk about potential applications as next-generation robotic stress sensors.

Skeletal muscles: modeling and simulation

Nilima Nigam (Simon Fraser University, Canada)

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Collaborators: Dr. James Wakeling

Skeletal muscles exhibit fascinating structural and mechanical properties. Skeletal muscle is composed of cells collectively referred to as fibers , which themselves contain contractile proteins arranged longtitudinally into sarcomeres. These latter respond to signals from the nervous system, and contract; unlike cardiac muscle, skeletal muscles can respond to voluntary control. Muscles react to mechanical forces - they contain connective tissue and fluid, and are linked via tendons to the skeletal system - but they also are capable of activation via stimulation (and hence, contraction) of the sacromeres. The restorative along-fibre force introduce strong mechanical anisotropy, and depend on departures from a characteristic length of the sarcomeres; diseases such as cerebral palsy cause this characteristic length to change, thereby impacting muscle force.

In the 1910s, A.V. Hill observed muscles heat when they contract, but not when they relax. Based on experiments on frogs he posited a mathematical description of skeletal muscles which approximated muscle as a 1-dimensional nonlinear and massless spring. This has been a remarkably successful model, and remains in wide use. Yet skeletal muscle is three dimensional, has mass, and a fairly complicated structure. Are these features important? What insights are gained if we include some of this complexity in our models? Mathematical questions of interest in skeletal muscle mechanics arise: how to model this system, and how to discretize it?

In this talk, we survey recent work on the modeling, simulation and validation of a fully 3-dimensional continuum elasticity approach for skeletal muscle dynamics. Skeletal muscle is modelled as a fibre-reinforced nonlinear elastic material, with other connective tissues such as aponeurosis and tendon being similarly described. These fibres are capable of nonlinear activation. We use a three-field formulation originally due to Simo and Taylor. After discretization (semi-implicit in time, FEM in space), the model is validated against physiological data, and then used to understand the impact of muscle architecture, mass and tissue properties on questions of physiological interest.

This is joint work based on a long-standing collaboration with James Wakeling (Dept. of Biomedical Physiology and Kinesiology, SFU), and several of our amazing students.

Mathematical methods and artificial intelligence in climate science

Terence O'Kane (Commonwealth Scientific and Industrial Research Organisation (CSIRO))

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Understanding and predicting the Earth's climate requires mathematical models governing the complex interplay between a diverse range of physical processes. These interactions span a huge range of spatial and temporal scales, from daily weather events, to the seasons, to multi-year climate variability (e.g. El Nino / La Nina cycle), and multi-decade climate change. Significant improvements have been made in weather forecasting with the advent of super computers, ready access to satellite data, in concert with mathematical advances in data assimilation and numerical methods. With its immediate impact on our daily lives, weather prediction is truly one of mankind's greatest achievements. However, modelling the climate on timescales of seasons to decades poses an even greater and arguably existential challenge. This talk gathers contributions from mathematics and artificial intelligence to highlight the challenges, latest developments, and current research questions to understanding the dynamics of the climate system. Emphasis is placed on the importance of developing quantitative methods to convey physical climate risk accounting for uncertainties in our observational record and the limitations of our modelling systems and theoretical underpinnings.

What do we need in a computational physiology framework to predict single cell biology?

Vijay Rajagopal (University of Melbourne)

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Cell biology is experiencing a big-data explosion with probes and microscopes now able to measure the physiological state of cells at single organelle resolution. New mathematical models, and innovations in multiscale computational modelling are needed to make sense of these rich datasets. In this talk we will describe new biophysics-based multi-scale models of calcium signalling, cell-cell adhesion, and energy metabolism. We highlight new knowledge that these models generate about the inner workings of living cells.

Mathematical theory of structured deep neural networks

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Deep learning has been widely applied and brought breakthroughs in speech recognition, computer vision, natural language processing, and many other domains. The involved deep neural network architectures and computational issues have been well studied in machine learning. But there is much less theoretical understanding about the modelling, approximation or generalization abilities of deep learning models with network architectures. An important family of structured deep neural networks is deep convolutional neural networks (CNNs) induced by convolutions. The convolutional architecture gives essential differences between deep CNNs and fully-connected neural networks, and the classical approximation theory for fully-connected networks developed around 30 years ago does not apply. This talk describes approximation and generalization analysis of deep CNNs and related structured deep neural networks.

General Communications

Organisers: Verónica Anaya, Ricardo Ruiz Baier

* * *

Finite element approximation for the unsteady Brinkman – Forchheimer equations

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We propose and analyse an augmented mixed formulation for the time-dependent Brinkman - Forchheimer equations written in terms of vorticity, velocity and pressure. We establish existence and uniqueness of a solution to the weak formulation, and derive the corresponding stability bounds, employing classical results on nonlinear monotone operators. Then, we propose a semi-discrete approximation based on stable Stokes elements for the velocity and pressure, and continuous or discontinuous piecewise polynomial spaces for the vorticity. In addition, by means of the backward Euler time discretisation, we introduce a fully discrete finite element scheme. We prove well-posedness and derive the stability bounds for both schemes, and establish the corresponding error estimates. We provide some numerical results verifying the theoretical rates of convergence.

Modelling coupled particle/air flow in industrial turbomachinery devices using a ghost cell immersed boundary method

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Collaborators: Paul W. Cleary, Matthew D. Sinnott

Understanding air flow in turbomachinery is important, particularly when it is used for transportation and/or processing of airborne granular materials. Optimal airflow ensures peak performance and efficiency as well as safeguarding equipment, reducing wear and the risk of mechanical failure. Predicting coupled airflow accurately within turbomachinery, however, presents significant challenges. These devices combine fast moving components like rotors and blades with stationary components like baffles, screens and housings. Further complicating matters, components often have fine scale intricate features (e.g., small perforations in screens) and narrow clearances between moving parts. The primary modelling challenges are to faithfully represent these geometrically intricate systems which encompass a broad range of length scales with narrow approaches between stationary and dynamic components. Then to devise robust computational algorithms that allow accurate prediction of how the air flow responds to components. Slip/sliding mesh methods are unviable as they cannot effectively resolve the large velocity gradients within the narrow clearances between the components. Immersed boundary methods (IB) are a promising alternative as they represent the components without the air having to conform to the component (solid) boundaries. The choice of IB variant, however, is important for our turbomachinery applications. Continuum forcing IB methods (where the influence of the solid boundary on the air flow is represented as a body force on the air), while easy to implement, do not guarantee correct enforcement of solid boundary conditions leading to erroneous mass fluxes through boundaries. The cut cell IB method, which modifies the discretised equations near the solid boundary, is too complicated for our geometries. Accordingly, we present a ghost cell IB method that employs elegant masking strategies to represent the changing geometry on a Cartesian grid. This IB method can be applied to any geometry that can be represented by a triangulated mesh. This is combined with a pressure-projection method to model the incompressible air flow and with the Discrete Element Method (DEM) to model the two-way interaction between particles and airflow for a broad range of particle shapes and sizes. The result is an inherently general capability to simulate fully coupled particle/air flow in complex industrial turbomachinery devices with narrow clearances.

Mass-conserving immersed boundary method for coupled incompressible solvers on collocated finite volume grids

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Collaborators: Nicholas Williamson, Steven W. Armfield

In computational fluid dynamics applications that contain complex geometries, mesh generation can be a very time consuming process. Furthermore, robust meshing algorithms which can deal with general geometries are not simple and require considerable programming effort. Ghost cell immersed boundary methods allow the solution of flows over arbitrary geometries on Cartesian grids, and are relatively easy to implement into an existing code. However, these methods do not conserve mass globally, even in a mass-conservative finite volume framework. The treatment of solid boundaries with corners is also difficult. Furthermore, when used with coupled solvers on collocated grids, correct implementation of momentum weighted interpolation at the boundaries is not straightforward. The approach presented here overcomes these issues by combining a directional ghost cell method with a weighted face flux correction based on the global mass continuity error. The method only requires the addition of source terms to the discrete equations. We have applied the technique in a fully coupled FAS multigrid scheme where the immersed boundary is solved on all grid levels. Performance and accuracy comparisons are made with the SIMPLE scheme in OpenFOAM using an unstructured mesh.

A complex-projected Rayleigh quotient iteration for targeting interior eigenvalues

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Collaborators: Nils Friess and Robert Scheichl (University of Heidelberg)

I will introduce a new "Projected Rayleigh Quotient Iteration" for computing an eigenvalue of a Hermitian matrix, which uses approximate eigenvector information to target interior eigenvalues and which is particularly suited to problems where the target eigenvalue has close neighbours. While classic Rayleigh quotient iteration converges locally very fast (cubically), its global convergence can be unpredictable, whereby it may not converge to the target eigenvalue or even the eigenvalue closest to the initial shift. This problem is greatly exacerbated when the eigenvalues are closely spaced. The key idea of the new algorithm is to utilise approximate eigenvector at each step by adding a complex-valued projection to the original matrix, such that the unwanted eigenvalues are lifted into the complex plane, while the target eigenvalue stays close to the real line. Thus, artificially increasing the distance between the target eigenvalue and the rest of the spectrum. I will present an error analysis of our new method, proving that under certain conditions our new method also converges cubically, and I will present several numerical examples demonstrating the improved global convergence behaviour. In one particular example we apply it to compute eigenvalues in a band-gap spectrum of a Sturm–Liouville operator used to model photonic crystal fibres, where the target and unwanted eigenvalues are closely spaced. The examples show that the new method converges to the desired eigenpair even when the eigenvalue spacing is very small, often succeeding when classic RQI fails.

A fast high order algorithm for multiple scattering from large configurations of scatterers

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Collaborators: M. Ganesh

Simulation of wave interactions with configurations containing large numbers of individual particles are important in diverse applications including oceanography and atmospheric science applications. Simulations need to account for reflections between all particles, the number of which grows with the square of the number of particles. Consequently, such simulations have been mostly limited to relatively small numbers of particles. We present an efficient solver based on a Krylov subspace method combined with a fast algorithm for computing matrix vector products whose complexity (memory and CPU time) grows only linearly with the number of particles. Our matrix vector product scheme is based on a novel numerically stable expansion of the field radiated by each particle in cylindrical or spherical wave functions. We demonstrate our algorithm by simulating multiple scattering for large configurations with tens or hundreds of thousands of individual particles.

The impacts of mortality rate and strong Allee effect in a three-species food chain model with Crowley-Martin functional response

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Collaborators: Siti Nurnabihah Karim, Hamizah Mohd Safuan, Sze Qi Chan

In the realm of ecology, strong Allee effect is closely associated with population sustainability to extinction. To address this topic, we propose and investigate the intricate features of a three-species food chain model subjected to Crowley-Martin functional response and strong Allee effect in prey species. Here, our focus is on how the mortality rate of middle predator can influence the interactions among species. For this purpose, numerical simulations and stability analysis are utilised to demonstrate the dynamics of the proposed model. The stability analysis is performed using linearization and eigenvalue methods on each equilibrium point. Through bifurcation analysis, we observe the bi-stable behaviour in the system as well as the occurrences of Hopf and transcritical bifurcations. It is worth noting that all three species maintain their viability at a medium mortality rate, whereas extinction occurs at a low mortality rate.

Using ODEs to solve an evolving interface problem

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Collaborators: Pascal R. Buenzli and Matthew J. Simpson

Reaction–diffusion partial differential equations (PDEs) on evolving interfaces can pose challenges when solved numerically, requiring the development and implementation of advanced numerical schemes to ensure conservation and precision. When these types of PDEs are used to model the collective behaviour of individual entities, such as cells in biological systems, we can capture the same collective behaviour using a system of ordinary differential equations (ODEs) that model the evolution of each cell. These individual-based models that are derived from first principles tend to be easy to solve numerically, and can be shown to recover the same PDEs in the continuum limit. In this presentation, we apply this approach to the evolution of the tissue interface in tissue growth problems. Our discrete model represents the tissue interface as a chain of individual cells that interact mechanically and are assumed to generate a constant area of tissue per unit time. The continuum limit of our discrete model is a reaction–diffusion PDE that governs the evolution of cell density on the evolving interface. While solving the discrete model solving is straight forward, the continuum model requires different numerical schemes between low to high diffusivities. When comparing numerical results for the discrete and continuum models, we show that small systems of ODEs provide a good approximation of the continuum model for all diffusivities, and that when the system becomes slightly larger discrepancies are significantly reduced.

A spectral method for two-dimensional partial differential equations on irregular domains

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We present a spectral method for solving two-dimensional partial differential equations (PDEs) on irregular domains. The method utilises a least-squares projection approach to solve an over-determined system accounting for the PDE and the boundary conditions embedded in an enclosing rectangular domain. Numerical experiments demonstrate the method's versatility on a variety of problems, and also shed light on some of the technical challenges inherent in this approach.

Numerical inversion of the Laplace transform with application to modelling railway transition zones

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With increasing demands being placed upon rail networks, both in Australia and globally, there is ongoing research into the underlying mechanics in a bid to improve track infrastructure and minimise required maintenance. Particular attention is paid to places in the track where the foundation properties change abruptly, referred to astransition zones. Increased dynamic forces and plastic deformations create negative feedback loops at transition zones which cause them to degrade more quickly than other sections of track. Seeking a better understanding of the mechanics of these systems, we investigate solutions to the Euler-Bernoulli beam equation on viscoelastic foundation with piece-wise constant coefficients using the Laplace transform in time and undetermined coefficients in space. Even in the simplest case, the inverse Laplace transform cannot be performed analytically and a suitable numerical inversion must be performed. This talk discusses an application of Weeks' method - which approximates the solution using Laguerre functions - to perform the Laplace inversion within the context of this problem.

Compressible ocean waves generated by sudden seabed rise near a step-type topography

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Collaborators: Santu Das and Mike Meylan

We consider the propagation of tsunami waves generated by ground motion, and their subsequent scattering from a sudden change in bathymetry following linearised water wave theory and a weakly compressible ocean. This talk presents a process of using eigenfunction matching to find solutions for an arbitrary piecewise-constant bathymetry profile in both the two-dimensional and axisymmetric three-dimensional cases. Numerical challengers are highlighted in the case of ground motion within an oceanic trench.

An exponential integration constraint energy minimizing generalized multiscale method for parabolic problems

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Collaborators: Juan Galvis and Eric T. Chung

This work investigates an efficient exponential integrator generalized multiscale finite element method for solving a class of time-evolving partial differential equations in bounded domains. The proposed method, known for its efficiency, first performs the spatial discretization of the model problem using constraint energy minimizing generalized multiscale finite element method (CEM-GMsFEM). This approach consists of two stages. First, the auxiliary space is constructed by solving local spectral problems, where the basis functions corresponding to small eigenvalues are captured. The multiscale basis functions are obtained in the second stage using the auxiliary space by solving local energy minimization problems over the oversampling domains. The basis functions have exponential decay outside the corresponding local oversampling regions. We shall regard the first and second-order explicit exponential Runge-Kutta approach for temporal discretization and to build a fully discrete numerical solution. The exponential integration strategy for the time variable allows us to take full advantage of the CEM-GMsFEM as it enables larger time steps due to its stability properties. We derive the error estimates in the energy norm under the regularity assumption. Finally, we will provide some numerical experiments to sustain the efficiency of the proposed method.

Stable dual pairing summation-by-parts operator for sediment transport model with well-posed boundary conditions

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Collaborators: Stephen Roberts, Kenneth Duru, Christoper Zoppou, Kenny Wiratama

Dual pairing summation-by-parts operator along with Godunov flux splitting that developed for the sediment transport model has been stably proven and weakly implemented using penalty. We identified the number of boundary conditions, location and form via energy method. Discrete-level stability was established using discrete energy estimate that mimics the continuous energy. The numerical experiments are presented to verify the analysis.

Linear and weakly nonlinear stability analyses in Horton-Rogers-Lapwood non-Newtonian nanofluid model

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Collaborators: Xinyi Zhu, Shilpi Agarwal

The classical Horton-Rogers-Lapwood (HRL) problem is extended for a non-Newtonian nanofluid-filled porous medium, subject to new hydrodynamic boundary conditions (rough boundaries) and isothermal boundary conditions. The key focus of the physical model lies in the modulation effects and a nonlinear Boussinesq approximation (maximum density property) for temperature and nanoparticle volume fraction in the buoyancy term of the momentum equation. This leads to a governing system comprising the continuity equation, the Navier–Stokes momentum equation, the equation of state, the energy equation, and the nanoparticle volume fraction equation. Linear stability analysis is performed after omitting the nonlinear interaction terms for rough boundaries and considering limiting cases: free-free, rigid-free, and rigid-rigid boundary conditions. The resulting eigenvalue problem is solved using an efficient numerical technique, and artificial neural network analysis is performed to express the relationship between the Rayleigh critical number and the relevant controlling parameters based on the numerical dataset. An optimal training algorithm is utilized, ensuring a low RMSE and a high R^2. A Lorenz equation system is derived using the spectral Fourier method for isothermal tangential stress-free boundary conditions. Additionally, weakly nonlinear stability analysis is conducted to quantify both heat and nanoparticle transport in the system, demonstrating the transition from periodic convection to chaotic convection and bifurcation.

Finite element method for a micromagnetic model at elevated temperatures

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The Landau–Lifshitz–Bloch (LLB) equation is a vector-valued quasilinear PDE, which is commonly used in the theory of micromagnetism to model the effects of magnetic field on a ferromagnetic material at elevated temperatures. In this talk, I will discuss the LLB equation with spin-torques resulting from applied current. Well-posedness of the problem is derived and a fully-discrete numerical method to solve the problem is proposed. This scheme is energy-dissipative in the absence of current. Assuming certain regularity of the exact solution, an optimal order of convergence to the solution is obtained for the scheme. This is corroborated by several numerical simulations.

Optimising mesh refinement for the reaction-diffusion-convection equation using AFEM

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Adaptive finite element approaches for the convection dominated problem fall into two main categories when handling mesh refinement. The first category is where a specific mesh refinement is used to focus on an interior or boundary layer, which may not be known in advance. The second category is where the mesh refinement is achieved dynamically by estimating the error of the current solution and refining the elements that contribute the highest amount of the total estimated error, which requires an error estimator to be chosen. We introduce an error estimator for the local projection stabilisation approach to refine adaptively the finite element grid. In this paper we present a method for optimising mesh refinement by using the Adaptive Finite Element Method.

A dual pairing summation-by-parts finite difference framework for nonlinear conservation laws

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Collaborators: Kenneth Duru and Nathan Lee

Robust and stable high-order numerical methods for solving partial differential equations are attractive because they are efficient on modern and next generation hardware architectures. However, the design of provably stable numerical methods for nonlinear hyperbolic conservation laws poses a significant challenge, as initial attempts often result in crashes due to compounding numerical errors or the presence of undesirable numerical oscillations, which can pollute numerical simulations everywhere. Desirable high-order accurate methods for nonlinear PDEs must be robust (provably stable) and preserve several important system invariants. We present the dual-pairing (DP) and upwind summation-by-parts (SBP) finite difference (FD) framework for accurate and robust numerical approximations of nonlinear conservation laws. The DP SBP FD operators are a dual-pair of backward and forward FD stencils, which together preserve the SBP property. In addition, the DP SBP FD operators are designed to be upwind, that is they come with some built-in dissipation everywhere, as opposed to discontinuous Galerkin methods which can only induce dissipation through numerical fluxes acting at element interfaces. We combine the DP SBP operators with skew-symmetric and upwind flux splitting of nonlinear hyperbolic conservation laws. Our semi-discrete approximation is conservative and provably entropy-stable for arbitrary nonlinear hyperbolic conservation laws. We give specific examples using the in-viscid Burger's equation, nonlinear shallow water equations and compressible Euler equations of gas dynamics.

Towards a multi-scale model of sugarcane bagasse chemical pre-treatment using microCT imaging

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Collaborators: Ian Turner, Elliot Carr

Sugarcane bagasse is a woody, fibrous by-product of the sugar industry that is fermented into biofuel. A crucial part of the process is the chemical pre-treatment step, typically conducted under pressure at temperatures below the boiling point of the solvent. In this process, the complex lignocellulose undergoes hydrolysis into simpler molecules, more readily digestible by enzymes. We seek to understand the heat and mass transfer phenomena within the heterogeneous bagasse particles during this pre-treatment process, and how the flow of reactants is affected by the complex porous structures. We use microCT imaging to reveal these microstructures in three dimensions and characterise the particle in terms of solid fraction and local density. We then use these images directly to compute effective material properties (anisotropic thermal conductivity, for example) throughout the particle. Since computing these effective properties everywhere in the particle would be computationally intensive, we also propose a spectral clustering strategy to group similar regions of the particle together. The similarity matrix for this strategy is constructed based on fast-to-compute heuristics such as solid fraction and fibre angle. We show that the clustering strategy separates visibly distinct regions of the particle, and that the error incurred by assigning one effective conductivity to the whole cluster is small.

Mathematical Biology

Organisers: Anne Boschman, Mark Flegg

* * *

Numerical framework for a dengue model governed by fractional derivative with singular and non-singular kernels

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Collaborators: Amin Jajarmi and Dumitru Baleanu

A novel numerical method is formulated to solve the fractional model with three different fractional operators with singular and nonsingular kernels. For the singular operator, we consider the Caputo fractional derivative while for the nonsingular ones, we take into account the Caputo–Fabrizio (with exponential kernel) and the ABC (with Mittage-Leffler kernel), respectively. Stability and convergence of the proposed numerical method are analysed. Using these singular and nonsingular kernels, a mathematical model for dengue fever outbreak is examined, based on a system of fractional differential equations. The equilibrium points and stability of the new system are studied. We fit the fractional model with a real data outbreak on the Cape Verde Islands that occurred in 2009 for a period of three months by using singular or nonsingular kernels. Simulation results show that the proposed formalism with exponential kernel agrees well with the real data in the early stage of the epidemic while the Mittag-Leffler kernel fits the reality for the later part of the time interval. Hence, the new framework in a hybrid manner can properly simulate the dynamics of the disease in the whole of the time interval. In order to stabilize the disease-free equilibrium point of the system under investigation, two control strategies are suggested. Numerical simulations verify that the proposed stabilizing controllers are efficient and provide significantly remarkable results.

Developments in stochastic reaction-diffusion algorithms

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Reaction-diffusion processes are important in various areas of science, particularly where large molecules are involved. In mathematical biology, these processes are often affected by their stochastic nature. An important goal in mathematical biology is whole-cell simulation (the simulation of a biological cell as a chemical system). Whilst whole-cell simulation has been achieved, spatially accurate stochastic models of whole cells have not been achieved and this is because of the immense computational challenges involved in simulating stochastic reaction-diffusion at the necessary scales. In this talk, I will walk through some of the important new finds in this area and some open challenges.

Jump-Switch-Flow: hybrid deterministic-stochastic trajectories of compartmental systems

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Collaborators: Alexander Zarebski, Sophie Hautphenne, Rob Moss, Jennifer Flegg, and Mark Flegg

Many dynamical systems exhibit multiscale behaviour. A classic example of this is the atto-fox problem in the Lotka-Volterra predator-prey model where oscillations lead to populations becoming unfeasibly small. Similar issues arise in epidemiology, immunology, and molecular biology, where small populations may go extinct due to stochastic effects. One resolution is to represent the process as a continuous time Markov chain (CTMC) which accounts for the discrete nature of small populations. Unfortunately, for large populations, simulating this process is computationally intractable. We have developed a way to approximate the CTMC which preserves the discrete stochastic behaviour of small population sizes, and continuous deterministic behaviour of large populations. Depending on the state of the system, the process switches between stochastic (jumping) and deterministic (flowing) regimes. We call this approach 'Jump-Switch-Flow' (JSF). In addition to incorporating small population stochastic effects, our approach also has a natural notion of compartment extinction, providing a solution to Atto-type problems. Here, I will present JSF (an open-source package implementing this approximation) and demonstrate, through a simulation study of an epidemiological SIRS model with demography, that it reproduces much of the behaviour of current gold standard exact simulation techniques, while being substantially faster. I will also show, using synthetic data as a toy example, how JSF lets us discuss elimination scenarios under intervention. Finally, using clinical data of SARS-CoV-2 infections, I will demonstrate how JSF enables the analysis of within-host processes, while accounting for viral clearance.

Block structured adaptive mesh refinement immersed boundary-lattice Boltzmann method and applications in flapping-wing and engineering flows

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Collaborators: Gerald Pereira

The lattice Boltzmann method (LBM) is a popular alternative to simulate flows in a low Mach number regime, due to its intrinsic parallelisation, simplicity, and efficiency. In the LBM, the Navier-Stokes equations are solved by the streaming and collision steps, where solving the Poisson equation is avoided. In this work, the no-slip boundary condition of solid objects is achieved by the immersed boundary method (IBM), where the fluid mesh does not need to conform to the surface of the solid object. The adaptive mesh refinement (AMR) is used to achieve the high accuracy and efficiency by generating the finer grids near the solid surface and coarser grids away from the solid surface. Then this IB-LBM numerical codes are applied to study the aerodynamics of flapping wings and flows in several engineering designs requiring AMR. Results show that the current numerical code based on IB-LBM can be used to study and solve the flows involving the moving object in a large amplitude.

Hybrid and Polytopal Methods

Organisers: David Mora, Jai Tushar

* * *

Analysis of LDG method for non-linear fractional Rayleigh–Stokes problem with variable coefficient on the non-uniform mesh

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Collaborators: D. N. Pandey

We study the fractional order Rayleigh–Stokes problem with variable coefficient in two dimensional, where the time-fractional derivative is considered in the sense of Caputo with order $\alpha \in (0, 1)$. Using the Faedo-Galerkin method, we first discuss the existence and uniqueness of weak solutions then we analyze the problem through the fully discrete scheme, utilizing finite differences in time and the local discontinuous Galerkin (LDG) method in space. We approximate the Caputo time-fractional derivative on the non-uniform (graded) mesh using the L1 scheme to handle the weak singularity of the solution. Finally, we present a few numerical tests that demonstrate the effectiveness of the approach and validate the validity of the underlying science.

Stabilization-Free VEM Part II: Construction details and higher-order schemes

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Collaborators: Moreno Pintore

In this presentation, we introduce and analyze a stabilization-free high-order Virtual Element Method (VEM) for solving two-dimensional second-order elliptic equations. The key feature of this method is the introduction of novel polynomial projections that enable the construction of structure-preserving schemes, eliminating the need for traditional stabilization techniques. We provide both necessary and sufficient conditions on the polynomial projection space to ensure the well-posedness of the scheme, as well as optimal a priori error estimates.

In the context of VEM discretization, stabilization has been a central topic of research, as evidenced by numerous recent studies. For example, stabilization terms are addressed through a reduced basis approach in previous works, and bounds for stability terms in a posteriori error analysis have been explored. Additionally, quantitative studies have examined the parameters involved in stabilization, and sensitivity analyses have highlighted the impact of variable parameters in eigenvalue problem solutions.

However, stabilization-free VEMs are gaining increasing attention in applications, especially in problems involving non-isotropic diffusive operators. These methods offer improved accuracy, particularly in the L^2 norm, making them attractive for a wide range of applications.

In this talk, we will provide a detailed explanation of the construction and implementation of the stabilization-free VEM scheme. We will also discuss its robustness, particularly in addressing problems with anisotropies. Several numerical experiments will be presented to demonstrate the stability of the method and its effectiveness in solving complex problems characterized by anisotropic diffusion.

On a virtual element method for the acoustic eigenvalue problem

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Collaborators: Linda Alzaben, Andreas Dedner, Lucia Gastaldi

In this talk I will revisit a VEM scheme for the approximation of the acoustic eigenvalue problem. Also in view of recent results on the approximation of parametric eigenvalue problems, we discuss the influence of the stabilising term on the results. It is shown rigorously that in some cases the stabilisation is not needed for the correct approximation of the eigensolutions.

Stabilization-Free VEM Part I: primal and mixed lowest order methods

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Collaborators: Stefano Berrone, Carlo Lovadina, Francesca Marcon, Gioana Teora and Michele Visinoni

In the framework of polygonal and polyhedral methods for the solution of partial differential equations, Virtual Element Methods (VEM) play a central role, since they enlarge the class of shapes that can be used in the computational mesh and thus increase the flexibility in handling geometrically complex domains. VEM schemes are based on the definition of local spaces of functions whose analytical expression is not known and suitable polynomial projections of basis functions are used to build consistent discrete bilinear forms, while coercivity is attained introducing a stabilizing operator. In this talk we introduce a new flavour of VEM in primal and mixed form, designed to avoid the use of an arbitrary stabilization term by making use of projections of basis functions on polynomial spaces of high degree. These methods preserve the structure of the exact bilinear form and are thus particularly suitable for the solution of problems characterized by anisotropies. We show some theoretical results about the well-posedness of the numerical scheme and display some numerical results highlighting the main features of the method.

Design and analysis of an extended virtual element method

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Collaborators: Gianmarco Manzini (Los Alamos National Laboratory) and Liam Yemm (Monash University)

The virtual element method (VEM) is now a well-established polytopal method, a numerical method to approximate solutions of partial differential equations on generic polygonal/polyhedral meshes. As usual in numerical approximation, the accuracy of the method is dictated in particular by the smoothness of the solution to the continuous problem. In complex geometries, one expects this solution to display reduced accuracy due to the geometric singularities of the domain. For a range of models, these singularities can however be analytically described. In that case, a way to recover optimal convergence rate consists in adding to the space of numerical approximation the singularity itself, so that the scheme can exactly reproduce it and only has to actually approximate the (smooth) remaining part of the solution. This approach has been developed at the end of the 90's for finite element schemes. These however lack the mesh flexibility of polytopal methods, which is in particular of interest when one needs to mesh domains with complex geometries. In this talk I will present an extended VEM, which consists in enriching the discrete approximation space with weak singularities. I will explain how the method is designed, and show that it recovers optimal approximation rates where the standard VEM accuracy is strongly limited by the smoothness of the solution. I will also discuss the proof of the error estimates, by explaining the roadblocks faced when attempting a "usual" VEM approach to the analysis and by showing that these roadblocks are overcome when employing a "fully discrete" approach (in the spirit of the analysis of the Hybrid High-Order method).

How flexible are the element shapes for VEM?

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Collaborators: Chunyu Chen and Huayi Wei

Virtual element methods have the advantages of being used on quite general (almost) arbitrarily polytopal-shaped meshes. For instance, small edges and small faces can be allowed. In this talk, we will present some recent progress on describing how flexible those polytopal elements can be under the framework of VEMs. We shall make an effort to generalize the well-known maximal angle conditions from simplicial meshes to polygonal meshes such that even shrinking elements can be also allowed. We will also discuss how solutions's regularity can affect the element shape.

DG-DGLM method and linear solver for hyperbolic conservation laws

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An arbitrary order discontinuous Galerkin method in space and time is proposed to approximate the solution to multi-dimensional hyperbolic conservation laws. Lagrange Multiplier is introduced on the edges of the element.

Weak formulation is derived through the definition of weak divergence. Lagrange multiplier is characterized as the average of the solutions on the edge. Stability and the error analysis are given. An edgewise iterative scheme is developed for the discrete system. Several numerical examples are presented.

Hybrid high-order methods for the wave equation in first-order form

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We discuss time-continuous and time-discrete schemes applied to the first-order formulation of the acoustic wave equation proposed and numerically investigated in [E. Burman *et al.*, 2022]. We employ explicit Runge-Kutta (ERK) schemes for the time discretization and hybrid high-order (HHO) method for the space discretization. We propose two general assumptions (I1)-(I2) for the interpolation operator, discuss corresponding consistency error, and present error analysis in this abstract setting. Interestingly, we consider altogether three interpolation operators depending on the setting (equal- vs. mixed-order, simplicial vs. polyhedral meshes), and two of these operators come from the hybridizable discontinuous Galerkin (HDG) literature. This illustrates the mutual benefits promoted by building bridges among methods. The key observation in the fully-discrete analysis is that it becomes crucial to bound the consistency error in space produced at each time step by measure of the stabilization seminorm only, and not the full HHO norm. With the help of three main properties (A1)-(A3), we prove that under specific CFL conditions subject to the s-stage ERK scheme, the method converges with predicted rates. The abstract template facilitates the application of our analysis to other non-conforming hybrid methods such as HDG and WG.

Hybrid high-order methods for extended Fisher-Kolmogorov and Fisher-Kolmogorov equation

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Collaborators: Neela Nataraj

This article analyzes the hybrid high-order methods for space discretization and backward Euler and Crank-Nicolson time discretization schemes for time discretization of extended Fisher Kolmogorov equations. The critical parameter $\gamma \geq 0$ is incorporated in the stabilization term of the HHO method. The analysis recovers the results for Fisher-Kolomogorov equations, that is, the case when the critical parameter $\gamma = 0$. The HHO space discretization and backward Euler (resp. Crank-Nicolson) time discretization lead to estimates of $O(h^{k+1} + \Delta t)$ (resp. $O(h^{k+1} + (\Delta t)^2)$ for the energy-norm when polynomials of order $k \geq 0$ are utilized to approximate normal derivative on the mesh faces. Moreover, the HHO discretization for Fisher-Kolmogorov equation ($\gamma = 0$) leads to convergence rate of $O(h^{k+2})$ in the space variable. The results of the numerical experiments validate the theoretical results.

Stream virtual element methods for the Navier-Stokes equations with pressure recovery

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Collaborators: Alberth Silgado

In this talk, we consider the two dimensional Navier-Stokes equations. We write a weak formulation in terms of the stream function of the velocity field. Next, we propose C^1-virtual element methods to discretize this formulation. Moreover, algorithms to compute the velocity, pressure and vorticity fields as a postprocess of the discrete stream function are proposed. Finally, we report several numerical experiments on different polygonal meshes.

Some new staggered DG methods on polygonal meshes

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The Staggered Discontinuous Galerkin (SDG) method is a numerical approach for solving partial differential equations, particularly on complex meshes like polygonal or polyhedral grids. The method is based on a mixed formulation along with staggered arrangement of primal and dual grids, which enhances stability and ensures local conservation of fluxes. SDG is known for its flexibility in handling various types of geometries and its ability to deliver accurate results without requiring stabilization techniques. This method has been successfully applied to problems in areas like fluid dynamics, electromagnetics, and structural mechanics.

In this talk, we briefly review our contributions on SDG and introduce some of the new SDG spaces, and discuss relations with existing polytopal element methods.

A discrete de Rham method for Einstein's equations

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There are many challenges to overcome when trying to numerically simulate Einstein's equations. In this talk we propose a discrete de Rham scheme for a recent 3+1 exterior calculus formulation of Einstein's equations, of which little is known about the theoretical properties so far. The method preserves exactly the constraints linked to the tetrad of the metric, but not necessarily the Hamiltonian constraint that should come as a result of the twice contracted Bianchi identities. Numerical results are discussed.

A C0 interior penalty method for mth-Laplace equation

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Collaborators: Huangxin Chen and Jingzhi Li

In this presentation, we propose a C0 interior penalty method for mTh-Laplace equation on bounded Lipschitz polyhedral domain in Rd, where m and d can be any positive integers. The standard H1-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. 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. The error estimate under the low regularity assumption of the exact solution is also obtained.

A posteriori error analysis of robust virtual element methods for stress-assisted diffusion problems

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Collaborators: Franco Dassi, Rekha Khot and Ricardo Ruiz Baier

In this paper, we develop and analyse upper and lower a posteriori error estimates for the virtual element discretisation of a nonlinear diffusion-elasticity coupled problem. The equations model stress-assisted diffusion and are of relevance, for example, in the electromechanics of soft tissues and simplified models for lithium-ion batteries. The error estimates are based on appropriately weighted norms that make the analysis robust with respect to model parameters. The a posteriori error estimators are of residual type (including also stabilisation terms), and their analysis requires modified projection and interpolation operators. The reliability bounds for the decoupled elasticity equations in mixed form follow from a parameter-robust global inf-sup condition and the properties of the modified projections, interpolations, and stabilisations. For the nonlinear diffusion in mixed form, we require in addition a Helmholtz decomposition and additional regularity of the boundary data. We provide several numerical experiments to demonstrate the sharpness of the error estimates in 2D and 3D problems.

Serendipity discrete complexes with enhanced regularity

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We address the problem of finding serendipity versions of approximate de Rham complexes with enhanced regularity. The starting point is a new abstract construction of general scope that, given three complexes linked by extension and reduction maps, generates a fourth complex with cohomology isomorphic to the former three. This construction is used to devise new serendipity versions of rot-rot and Stokes complexes derived in the Discrete de Rham spirit.

A discrete trace theory for non-conforming polytopal hybrid discretisation methods

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We discuss a discrete trace theory for non-conforming hybrid methods that holds on polytopal meshes. A notion of a discrete trace seminorm is defined, and *trace* and *lifting* results with respect to a discrete H^1-seminorm on the hybrid fully discrete space are proven. We also discuss a numerical test in which we compute the operators associated with the proposed norms and show that their spectrums are equivalent, verifying the theoretical analysis. The development of this theory is motivated by the design and analysis of preconditioners for hybrid methods, e.g., of substructuring domain decomposition type.

Mathematics of Machine Learning

Organisers: Vinesha Peiris, Sergio Rojas

* * *

A posteriori error estimates and adaptive mesh refinement for variational physics informed neural networks

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Collaborators: Moreno Pintore

In this talk, we introduce a meshfree Variational-Physics-Informed Neural Network (VPINN), which eliminates the need for domain triangulation and allows training with an adaptive set of test functions. We propose a computable residual-type a posteriori error estimator to control the energy error between the exact solution and the VPINN solution. Our estimator is both reliable and efficient, as it provides upper and lower bounds for the global error in terms of a constant multiple of the estimator, up to data oscillation terms.

Reliability ensures that the global error is controlled, enabling adaptive refinement of the test space by adding test functions in regions where the estimator is large, thus improving accuracy. Efficiency allows for coarsening the test space by removing test functions in regions with small error, optimising computational resources.

The estimator consists of several components, including a classical residual-type estimator that measures the residual of the strong form of the differential equation when the VPINN solution is substituted. It also includes terms related to the loss function magnitude post-minimisation and additional terms for data oscillations, arising from the projection of the equation's coefficients and right-hand side onto polynomial spaces. The estimator can be locally decomposed, making it suitable for adaptive discretisation strategies where elements contributing most to the estimator are refined.

Additionally, we propose four training strategies for the meshfree VPINN and compare them with standard VPINN methods. Numerical results demonstrate that our approach achieves higher accuracy than a quasi-uniformly meshed VPINN trained with the same number of test functions, showing the effectiveness of adaptive test function selection in improving solution precision.

Universal monotonic flow-based generative models via latent dynamics

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Flow-based generative models such as normalizing flows parametrize bijective mappings between the base distribution and the target distribution. These models are able to learn complex distributions and allow rapid generation. However, the design of the flow architecture is a challenging task due to the requirement on bijection, expressive power, computational efficiency. In this talk, we present a novel monotonic normalizing flow model called AUTM. It employs a latent variable to facilitate the inverse transformation and the flow can be shown to be universal. Computationally, AUTM allows straightforward calculation of Jacobian determinant during training. Experiments on large scale data sets demonstrate the advantages of AUTM over other flow models.

Adaptive fuzzy inference system-based deep learning model for software dependability analysis

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Collaborators: Deepjyoti Saha

In the era of advanced technology, predicting various dependability attributes such as reliability, security, maintainability, and availability and analysing their impact on overall software systems during the early phases of software development are very challenging task due to the increased complexity and scale of modern software systems. To address these challenges, various data-driven models have been developed recently for fault and vulnerability prediction during the early phase. However, many of these approaches fail to account for analysing the impact of dependability attributes on the overall system. To overcome this limitation, this paper proposes a fuzzified model for predicting multiple dependability attributes early in the development process. Fuzzy logic is employed in this article to handle imprecise and uncertain software metrics and predict various dependability attributes by converting inputs into fuzzy membership values and applying expert-driven if-then rules to account for uncertainty. Additionally, a deep neural network model is developed to categorize between dependable and non-dependable software modules by identifying complex patterns in the predicted attribute values. The combination of fuzzy logic and deep learning offers a more adaptive and comprehensive approach for software dependability analysis during early in the software development lifecycle. This methodology has been validated and compared with existing models using real datasets. The experiments demonstrates that the proposed model gives the superior performance. This proposed model enables informed decision-making, improved resource allocation, and early detection of risk-prone areas, leading to more reliable, maintainable, and secure software systems.

Leveraging machine learning for macroeconomic forecasting

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Background: Macroeconomic forecasting has historically relied on simple regression and time series techniques, which have often struggled to outperform basic benchmarks. In a study by Panagiotelis et al., 151 aggregate and disaggregate economic series, along with 185 international variables, were employed as predictors for an Australian macroeconomic model. The study found that expanding the model to include more than 20 variables, particularly international ones, did not significantly improve the accuracy of forecasts for Australian macroeconomic indicators.

Dataset: We incorporated 16 predictors identified from previous literature, focusing on Gross Domestic Product (GDP) growth, Consumer Price Index (CPI) inflation, and the Interbank Overnight Cash Rate (IBR). The dataset is composed of values of 19 indicators for each quarter from June 1985 to September 2023, with variables as in table 1.

Method: We apply a combination of ML and DL techniques to forecast key macroeconomic indicators for Australia. Model performance is evaluated against basic benchmarks, with the random walk (RW) model serving as the baseline. We employ ARIMAX as the time series method, RF and XGBoost as ML methods, and an ensemble of these two models. For DL methods, we utilize Long Short-Term Memory (LSTM), Convolutional Neural Network-LSTM (CNN-LSTM), and Feedforward Neural Networks (FNN). Model performance is assessed using Root Mean Squared Error (RMSE) and Mean Absolute Scaled Error (MASE).

Results: Our result shows better performance of ML methods. Ensemble ML methods of Random Forest (RF) and XGBoost deliver superior predictive performance, while DL methods did not achieve comparable accuracy in this context. The result is shown in Table 2.

Climate reduce-order modelling: Galerkin projection of the atmospheric equations of motion onto an orthogonal basis

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Collaborators: Laurent Cordier and Terence O'Kane

Weather forecasting is a BigData problem, with many relevant samples. Standard machine learning approaches make minimal assumptions of the underlying system, by using methods capable of capturing many forms of non-linearity with many parameters. In contrast climate projection is a SmallData problem, with few relevant samples due to the slow time scales, boundary conditions with trends (e.g. increasing greenhouse gas concentrations), and short observational period. Our general approach is to make maximal physical assumptions by allowing only the nonlinearity supported by the equations of motion, hence requiring far fewer parameters. We do so by developing a reduced-order model of the global atmosphere in which we symbolically project the hydrostatic equations of motion onto a set of empirical orthogonal functions (EOF). This approach transforms a system of partial differential equations dependent upon time and space, into a system of ordinary differential equations dependent upon time and EOF mode index. As such, one instead solves for the coupled temporal evolution of each principal component, as opposed to the spatio-temporal evolution of the field variables; representing a massive dimension reduction. The required three-dimensional EOF modes are calculated from the atmospheric fields of the ensemble climate reanalysis dataset, CAFE60, which comprises of 96 realisations of the Earth every day from 1960 to near present day. The reduced-order model coefficients are calculated by solving a regression problem in which the input factors are only those justified by the non-linearities encoded in the physical equations of motion. This approach delivers a reduced-order model that reproduces the large-scale atmospheric variability at a fraction of the computational cost required to numerically simulate the flow.

Compatible finite element interpolated neural networks

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We extend the finite element interpolated neural network (FEINN) framework from partial differential equations (PDEs) with weak solutions in H^1 space to PDEs with weak solutions in $H(\text{curl})$ or $H(\text{div})$ spaces. To this end, we consider interpolation trial spaces that satisfy the de Rham Hilbert subcomplex, providing stable and structure-preserving neural network discretisations for a wide variety of forward and inverse PDE problems. We call this new approach compatible FEINNs. We show that compatible FEINNs are able to accurately approximate Maxwell's equations: the trained networks outperform finite element solutions by several orders of magnitude for smooth analytical solutions, while matching finite element accuracy for singular solutions. Furthermore, to showcase the versatility of the method, we demonstrate that compatible FEINNs achieve high accuracy in solving surface PDEs such as the Darcy equation on a sphere. Additionally, the framework can integrate adaptive mesh refinements to effectively tackle Maxwell's equations with localised features. Finally, we compare compatible FEINNs with the adjoint neural network method for solving inverse problems, such as identifying space-varying physical parameters for the Maxwell problem from partial or noisy observations. We find that compatible FEINNs accomplish comparable, if not superior, accuracy and robustness in these scenarios.

Energy minimisation using tensor-product free-knot B-splines

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We present a general framework for the minimisation of energy functionals within parametric functional spaces, offering an alternative approach to standard adaptive procedures for solving PDEs with solutions exhibiting localised features such as singularities, sharp fronts, and multi-scale phenomena.

Our approach is based on parametric functional spaces formed by a collection of free patches obtained by tensor-product of one-dimensional patches. These patches can move freely across the domain, allowing for dynamic adaptation to the local behaviour of the solution. We specifically focus on free-knot B-splines and shallow neural networks, both of which naturally leverage the tensor-product structure to balance flexibility and computational efficiency. A key strength of our framework is its versatility, as it encompasses a broad range of functional spaces, including sparse grids.

We provide elements of the numerical analysis of our approach, highlighting its theoretical foundations and practical advantages over conventional techniques. We provide several representative numerical experiments to demonstrate the versatility and effectiveness of our method.

Bayesian structure learning for climate model evaluation

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A Bayesian structure learning approach is employed to compare and contrast interactions between the major climate teleconnections over the recent past as revealed in reanalyses and climate model simulations from leading Meteorological Centers. In a previous study, the authors demonstrated a general framework using homogeneous Dynamic Bayesian Network models constructed from reanalyzed time series of empirical climate indices to compare probabilistic graphical models. Reversible jump Markov Chain Monte Carlo is used to provide uncertainty quantification for selecting the respective network structures. The incorporation of confidence measures in structural features provided by the Bayesian approach is key to yielding informative measures of the differences between products if network-based approaches are to be used for model evaluation, particularly as point estimates alone may understate the relevant uncertainties. Here we compare models fitted from the NCEP/NCAR and JRA-55 reanalyses and Coupled Model Intercomparison Project version 5 (CMIP5) historical simulations in terms of associations for which there is high posterior confidence. Examination of differences in the posterior probabilities assigned to edges of the directed acyclic graph provides a quantitative summary of departures in the CMIP5 models from reanalyses. In general terms the climate model simulations are in better agreement with reanalyses where tropical processes dominate, and autocorrelation time scales are long. Seasonal effects are shown to be important when examining tropical-extratropical interactions with the greatest discrepancies and largest uncertainties present for the Southern Hemisphere teleconnections.

Kolmogorov-Arnold theorem and its applications

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Kolmogorov-Arnold representation theorem (KA theorem) states that every multivariate function can be represented by compositions and summations of univariate functions. Even though the KA theorem has been very well known since 1957, nobody is fully aware of how this function representation works. Therefore, this has been an unsolved problem for many decades. However, some modified versions of this theorem have similar structures as neural networks which are the building blocks of artificial intelligence, but these interpretations have been highly arguable for several years. In this talk, we walk through the history of the KA theorem, its relation to neural networks and recent developments in this area. We will focus on the latest advancement involving rational functions, approximation and optimisation techniques, highlighting their applications where dimension reduction is necessary.

Robust variational physics-informed neural networks

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Collaborators: Paweł Maczuga, Judit Muñoz-Matute, David Pardo, Maciej Paszyński

This talk introduces a Robust version of the Variational Physics-Informed Neural Networks method (RVPINNs). As in VPINNs, we define the quadratic loss functional in terms of a Petrov-Galerkin-type variational formulation of the PDE problem: the trial space is a (Deep) Neural Network (DNN) manifold, while the test space is a finite-dimensional vector space. Whereas the VPINN's loss depends upon the selected basis functions of a given test space, herein, we minimize a loss based on the discrete dual norm of the residual. The main advantage of such a loss definition is that it provides a reliable and efficient estimator of the true error in the energy norm under the assumption of the existence of a local Fortin operator. We test the performance and robustness of our algorithm in several advection-diffusion problems. These numerical results perfectly align with our theoretical findings, showing that our estimates are sharp.

Improving Thornley's Model and Investigating Identifiability of its Parameters

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Collaborators: Brodie Lawson (The ARC Centre of Excellence), and Kevin Burrage (University of Oxford)

Mathematical modelling is an important mechanism for predicting and optimising plant growth, and Thornley's mathematical model provides a useful and mechanistic description of carbon and nitrogen allocation in plants. However, the model has not been thoroughly investigated, especially for significant variations of its parameters. This model consists of six non-linear ordinary differential equations that describe the temporal dynamics of acquisition, consumption and transport of carbon and nitrogen. We identify a wide range of non-physical behaviours in the model, and so we modify the model using a physical argument to improve realism. We find that this modification results in a model that behaves more realistically, for example no longer exhibiting sustained oscillations in mass. We then use simulation and Bayesian inference to investigate parameter identifiability in the new model. After Bayesian calibration to synthetic data, we see that the parameters controlling carbon uptake and consumption are strongly constrained in fitting to the data, but only as a pair. The equivalent parameters for nitrogen are similar, but less strongly constrained. Also, our identifiability analysis confirms that the combination of all four parameters that defines steady state behaviour in the original Thornley's model remains fundamentally important in the modified model.

Numerical Analysis for Coupled Multiphysics Problems

Organisers: Ricardo Oyarzúa, Segundo Villa Fuentes

* * *

A mixed FEM for curve diffusion flow problem in one dimension using bi-orthogonal systems

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Collaborators: Bishnu Lamichhane and James McCoy

Diffusion processes are relevant for the kinetics of many micro-structural changes that occur during the preparation, processing, and heat treatment of materials such as annealing of metals. The curve diffusion flow is a specific fourth-order evolution law describing how a curve in the plane or space changes shape in time. We consider the finite element method (FEM) based on bi-orthogonal system to find approximate solutions to curve diffusion flow for closed curves. The structure of bi-orthogonal systems helps in controlling the error in the numerical solution. Since the basis functions are constructed to satisfy specific orthogonality requirements, which help in minimising the error. In this endeavour, we introduce an unknown variable to establish a mixed formulation of the problem and employ a constrained minimisation approach to shape our problem and the FEM. This formulation reduces the order of the problem, resulting in an efficient and straightforward numerical approximation. Subsequently, we derive semi-discrete schemes utilising piecewise linear finite elements in the spatial direction, transforming the fourth-order problem into a semi-discrete system of second-order problems that are discretised in time using the forward Euler method. As a result, we attain systems of linear equations that are solved at every time step.

A conforming mixed finite element method for a coupled Navier–Stokes and transport system modelling reverse osmosis

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We consider the coupled Navier-Stokes and transport equations with nonlinear transmission conditions, which are commonly used to simulate the reverse osmosis effect in water desalination processes involving coupled feed and permeate channels through a semi-permeable membrane. The variational formulation consists of equations where velocities, concentrations, and auxiliary tensors and vector fields, along with two Lagrange multipliers, are the main unknowns of the system. This leads to a mixed formulation based on Banach spaces with a perturbed saddle point structure. We analyse the continuous and discrete solvability of this problem by applying the Banach fixed point theorem together with the Banach-Nečas-Babuška result. For the discrete scheme, we identify suitable finite element subspaces that yield stable discrete schemes. Finally, numerical results illustrating the applicability of the scheme are presented.

Phase-field modelling of adhesive interfaces

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In biological systems, the evolution of material boundaries is often driven by complex processes at the interface, such as biofilm growth, or between two interfaces, as seen in cell-cell and cell-substrate adhesion. In this talk, I will present a thermomechanically-consistent model that describes adhesive interactions between interfaces within the phase-field framework. The model is based on an energy functional which includes terms that are restricted to the diffuse interfaces, resulting in a bulk-surface type of interaction. Through formal asymptotic analysis, I will show that steady states of the model can be characterized by exploiting the connection between sharp-interface and diffuse-interface approaches. To support this analysis, I will present numerical results and discuss the energy stability of the used scheme.

Frequency-domain formulation and convergence analysis of Biot's poroelasticity equations based on total pressure

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Collaborators: Alfonso Caiazzo, Felipe Galarce, Joaquin Mura

In this talk, we discuss the well-posedness and error analysis of the Biot's Poroelastic equations. To demonstrate the solvability of the poroelastic continuous issue, we first use the well-known Fredholm Alternative. In order to improve computational efficiency and address the issues raised by the discrete inf-sup condition, we present a novel and stable stabilized numerical system that is tuned for equal polynomial order. Additionally, we conduct a numerical analysis to determine the stability of solutions and provide an a priori error analysis. Finally, we present some numerical examples that offer strong evidence of the usefulness and effectiveness of the proposed numerical framework.

A fictitious domain approach for the finite element discretization of FSI

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Collaborators: Daniele Boffi, Fabio Credali and Najwa Alshehri

In this talk I present some recent advances on a fictitious domain approach for he discretization of fluid-structure interaction problems proposed in [1]. This formulation is based on the introduction of a distributed Lagrange multiplier so that the problem fits in the framework of saddle point systems and possible stable choices of the finite element spaces which have been investigated in [2]. Our formulation allows for solving the Navier-Stokes equation and the elasticity equation on meshes independent of each other, at the price of computing a coupling term which involves test funtions defined on both meshes. A discussion on how to deal carefully with such term will also be presented, see [3] and [4]. We shall show also that the formulation is robust with respect small cells.

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A posteriori error analysis of a mixed FEM for the stationary convective Brinkman–Forchheimer problem

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In this talk we consider a Banach spaces-based mixed variational formulation that has been recently proposed for the nonlinear problem given by the stationary convective Brinkman–Forchheimer equations, and develop a reliable and efficient residual-based a posteriori error estimator for the 2D and 3D versions of the associated mixed finite element scheme. For the reliability analysis, we utilize the global inf-sup condition of the problem, combined with appropriate small data assumptions, a stable Helmholtz decomposition in nonstandard Banach spaces, and the local approximation properties of the Raviart–Thomas and Clément interpolants. In turn, inverse inequalities, the localisation technique based on bubble functions in local L^p-spaces, and known results from previous works, are the main tools yielding the efficiency estimate. Finally, we show several numerical results confirming the theoretical properties of the estimator and illustrating the performance of the associated adaptive algorithm.

Recent advances in numerical approximations for optimal control of fluid flow problems

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This talk delves into the fascinating realm of fluid flow problems, highlighting recent theoretical advancements and numerical innovations. We will present minimal regularity results for the governing equations—results that hold significance well beyond the scope of this field. Following that, we will explore the H^{div}-conforming discontinuous Galerkin formulation, an advanced method designed to handle these intricate flows. Additionally, we will demonstrate the efficiency and reliability of residual-based a posteriori error estimators, ensuring precision at each stage. Finally, numerical results will confirm our theoretical findings and underscore the strength of adaptive solution algorithms driven by our novel error estimators.

Case wise study of surface waves in a hydrostatic stress magneto-elasticity composite model

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This article investigates the consequences of hydrostatic stress, magneto-elasticity, and transverse isotropy on Love wave, Rayleigh wave, and SH-wave propagation in a composite structure with different hydrostatic stresses and magnetic effects. Generalised Ohm's law and Maxwell's equations were considered to compute the Lorentz force used in the present mathematical model. Dispersion relations have been analytically derived for Love-wave, while dispersion equations have been formulated in closed form for SH-wave and Rayleigh wave, respectively. The dimensionless phase velocity of each surface wave is computed numerically and depicted graphically to manifest the dependency on the magneto-elasticity, hydrostatic stress, and frequency. Keywords: Love wave, Rayleigh Wave, SH-wave, Magneto-elasticity, Maxwell Equation, Lorentz's force

Smoothed particle hydrodynamics for simulating heat transfer with mixed boundary conditions

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In this study, heat transfer in thin plates is simulated by solving the 2D heat equation using the Smoothed Particle Hydrodynamics (SPH) method. The solutions are approximated for mixed boundary conditions namely nonhomogeneous Dirichlet and homogeneous Neumann. To validate the numerical scheme, the SPH solution is compared with analytical and finite element (FEM) solutions for one type of boundary condition. The small RMSE indicates that SPH is good at approaching the analytical solution. Then, SPH is used to study the effect of insulation and heat sources on heat distribution. The isolated cavity in the center of the plate causes heat to transfer more quickly. Between several heat source geometries with the same area, heat is transferred efficiently by the star shape. The success in the simulation shows the flexibility of SPH in approaching heat equation solutions with complex geometries and boundary conditions, which are difficult to solve analytically or using FEM.

A mixed finite element method for extended Fisher-Kolmogorov equation based on biorthogonal systems

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Collaborators: Avijit Das, Neela Nataraj

We introduce a mixed finite element framework based on a saddle-point formulation for an extended Fisher-Kolmogorov equation, which is a nonlinear time-dependent fourth order partial differential equation. We apply biorthogonal basis functions to get an efficient finite element approach. We also obtain optimal error estimates for the finite element solution. The numerical experiments validate the theoretical estimates.

Helmholtz preconditioning for multi-scale atmospheric dynamics

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Discrete representations of the compressible Euler equations for atmospheric motion allow for several different design choices. Collocating the thermodynamic variable with the vertical velocity ensures there are no spurious computational modes, however this choice breaks energy conservation. Conversely collocating the thermodynamic variable with the pressure allows for skew-symmetric formulations that conserve energy, but also supports a spurious computational mode. Moreover the thermodynamic variable may also be transported in either material or density weighted flux form. These different choices lead to different linearisations and scalings when developing Helmholtz preconditioners for implicit solvers. Here we compare the stability and convergence of different Helmholtz operators for different discretisations and representations of the potential temperature. We also present a novel preconditioner for an energy conserving flux form representation that allows the resulting preconditioner to scale with both the fast acoustic and buoyancy modes of a compressible stratified atmosphere by first performing a transformation into a secondary residual expression for the thermodynamic entropy. Idealised tests show that this new formulation exhibits improved stability and convergence with respect to either standard linearisations of the energy conserving system, or a discretisation free of computational modes. The new preconditioner is further verified against standard test cases for a stratified atmosphere within a vertical slice geometry.

Analysis of the staggered DG method for the quasi-Newtonian Stokes flows

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Collaborators: Yang Liu and Lina Zhao

In this talk, I will present a divergence-free staggered discontinuous Galerkin (DG) method for quasi-Newtonian Stokes flow problems. The flux and the tensor gradient of the velocity are introduced as additional unknowns and the pressure variable is eliminated from the system via the incompressibility condition. Thanks to the subtle construction of the finite element spaces used in our staggered DG method, no additional numerical flux or stabilization terms are needed. The well-posedness of this scheme is based on the abstract theory for the non-linear twofold saddle point problems. A prior error analysis for all the involved unknowns is also provided. In addition, the proposed scheme can be hybridizable and the global problem only involves the trace variables, rendering the method computationally attractive. Finally, several numerical experiments are carried out to illustrate the performance of our scheme.

Adsorption system topology optimisation

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Collaborators: Santiago Badia, Aaron Thornton and Matthew Hill

The performance of swing adsorption systems is sensitive to the geometry of the adsorbent. To achieve feasibility for large-scale implementation of CO_2 direct air capture systems in line with the latest intergovernmental panel on climate change objectives, significant improvements to current adsorption systems must be made. In this study, we employ a topology optimization to the macrostructure of a swing adsorption bed and unveil a simple blunted cone design, which achieves an estimated cost range of $49 - 116/t - CO_2$ removed from the atmosphere. This represents an improvement over the benchmark monolith design, which incurs a cost of $75 - 140/t - CO_2$ considering the same process parameters. By reimagining the bed configuration, we demonstrate the potential for enhanced efficiency in adsorption systems.

Scalable solvers for the inductionless Magneto-Hydrodynamics (MHD) equations at high Hartmann numbers

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Collaborators: Santiago Badia

The inductionless magnetohydrodynamics (MHD) equations describe the behavior of a conducting fluid in the presence of magnetic fields, in a regime where magnetic induction effects can be neglected. They are widely used in many real-life applications, such as the modeling of liquid lithium-lead breeding blankets for nuclear fusion reactors. This nonlinear system of PDEs is characterized by the presence of strong coupling terms between the fluid and magnetic variables, which poses significant challenges to the numerical solution of the MHD equations. We will present a new scalable Hartmann-robust solver that addresses such problems and maintains it's convergence properties for a wide range of the parameters. The discretisation of the system of PDEs relies on a stable finite element space for the fluid problem that locally preserves mass conservation and a compatible divergence-conforming finite element space for the magnetic problem that preserves divergence pointwise.

Multiscale models for nonlinear transient electromagnetic problems with confined eddy currents

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Heterogeneous materials and structures, such as coils, iron sheets and composites, are widespread in electrical engineering. But they lead to unaffordable costs for the computation of electromagnetic fields using the Finite Element Method (FEM).

This presentation is about the multiscale modeling of electromagnetic fields on heterogeneous materials with periodic geometries. The numerical method used is the Heterogeneous Multiscale Method (HMM), also known as FE^2 method, for solving homogenised Maxwell's equations.

The main contribution of this work is to introduce new homogenisation formulas for the magnetic field, making the homogenisation robust to the presence of strong locally confined induced currents, responsible for hysteresis in the homogenised material law. We illustrate why the magnetic field cannot always be homogenizsd using the usual volume average. The model is numerically validated on linear and non-linear 3D transient problems.

Analysis of a FEM with exactly divergence-free magnetic field for the stationary MHD problem

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In this work we analyse a mixed finite element method for the stationary incompressible magneto-hydrodynamic problem providing an exactly divergence-free approximation of the magnetic field and a direct approximation of the electric field. The method is based on the introduction of the electric field as a further unknown leading to a mixed formulation where the primary magnetic variables consist of the electric and the magnetic fields, and a Lagrange multiplier included to enforce the divergence-free constraint of the magnetic field, whereas the hydrodynamic unknowns are the velocity and pressure. Then the associated Galerkin scheme can be defined by employing Nédélec and Raviart–Thomas elements of lowest order for the electric and magnetic fields, respectively, discontinuous piecewise constants for the Lagrange multiplier and any inf-sup stable pair of elements for the velocity and pressure, such as the MINI-element.

A DEM numerical framework to model jamming gripper

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Collaborators: Gary Delaney, Richard Scalzo, Paul Cleary

This study presents a Discrete Element Method (DEM) framework for modelling the mechanical behaviour of jamming grippers, which leverage the jamming transition of granular material to conform around and securely grip objects. The DEM model captures the complex particle-scale interactions and dynamics of the jamming transition, where granular material shifts from a free-flowing to a rigid state. A key feature of this model is the use of superquadric particles to represent realistic particle shapes, providing enhanced realism in particle interactions. Additionally, a Bonded Particle Model (BPM) is incorporated to simulate the flexible membrane surrounding the granular material, allowing for modelling of membrane deformation and its influence on the jamming process. Aspects of the framework will be illustrated by selected examples, demonstrating the effects of particle shape and membrane flexibility on the jamming transition and grip performance. The study aims to provide valuable insights into the mechanics of jamming grippers, offering pathways to improve their design and enhance their performance in practical applications.

Thermodynamic consistency and structure-preservation in summation by parts methods for the moist compressible Euler equations

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Collaborators: David Lee, Kenneth Duru

Moist thermodynamics is a fundamental driver of atmospheric dynamics across all scales, making accurate modelling of these processes essential for reliable weather forecasts and climate change projections. However, atmospheric models often make a variety of inconsistent approximations in representing moist thermodynamics. These inconsistencies can introduce spurious sources and sinks of energy, potentially compromising the integrity of the models. Here, we present a thermodynamically consistent and structure preserving formulation of the moist compressible Euler equations. When discretised with any summation by parts method, our spatial discretisation conserves: mass, water, entropy, and energy. These properties are achieved by discretising a skew symmetric form of the moist Euler equations, using entropy as a prognostic variable, and the summation-by-parts property. Additionally, we derive a discontinuous Galerkin spectral element method with energy and tracer variance stable numerical fluxes, and experimentally verify our theoretical results through numerical simulations.

A residual-based a posteriori error estimator for a non-isothermal Navier-Stokes/Darcy coupled system

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In this work we propose a residual-based a posteriori error estimator for a conforming discretization of a nonisothermal Navier-Stokes/Darcy coupled system in two and three dimensions. More precisely, we introduce a reliable and efficient a posteriori error estimator the coupled system where the primal formulation of the convection-diffusion equation for the temperature, is coupled with the velocity-pressure formulation of the Navier-Stokes problem in the free-fluid region, and the dual-mixed velocity-pressure formulation of the Darcy equation in the porous medium domain. The latter, suggests the introduction of a Lagrange multiplier representing the Darcy pressure on the interface. The Galerkin scheme considers the Bernardi-Raugel and Raviart-Thomas elements for the velocities, piecewise constant elements for pressures, continuous piecewise linear functions for temperatures, and continuous piecewise linear functions for the Lagrange multiplier on a partition of the interface. Employing standard arguments such as global inf-sup conditions, suitable Helmholtz's decompositions and the local approximation properties of the Raviart-Thomas and Clément interpolation operators, we derive the a posteriori error estimator and prove its reliability. In turn, inverse inequalities, usual localization techniques of bubble functions and known results from previous works, are employed to prove the local efficiency of the proposed error estimator. Finally, we propose an adaptive algorithm based on the local and computable error indicators of the a posteriori error estimator and provide several numerical examples to illustrate its performance and effectiveness.

An efficient pseudospectral approximation of non-Linear time-evolution equations

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The persistent challenge of nonlinear equations in various scientific domains has encouraged continuous exploration of numerical techniques. We employ a collocation-based Chebyshev spectral method, utilising the Chebyshev Gauss-Lobatto (CGL) points, to approximate the nonlinear Burgers' equation. Through discretisation, the original nonlinear equation is transformed into a system of ordinary differential equations (ODEs), which are subsequently solved iteratively using the Runge-Kutta 4th-order method. Our numerical experiments demonstrate the efficacy and robustness of the proposed scheme surpass the existing results by a significant margin. This methodology offers a promising solution to nonlinear equations and a versatile framework applicable to diverse scientific problems.

Space–time energy and entropy conservation for the thermal shallow water equations

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Collaborators: Santiago Badia and David Lee

The thermal shallow water equations are a non-canonical Hamiltonian system endowed with energy preservation and invariant casimir functions. Conservation of buoyancy–related invariants bounds unstable growth associated with grid scale variance in numerical simulations, and is therefore a desirable property of state-of-the-art numerical solvers of Hamiltonian systems. Quadratic invariants, like energy, can be discretely conserved using a Poisson time integrator and a skew symmetric spatial discretisation. Buoyancy related invariants are cubic, and the extension of Poisson integrators to higher order invariants has not yet been explored.

In this study, we develop a novel space–time finite element discretisation of the thermal shallow water equations that provably conserves discrete energy and buoyancy–related invariants. Our approach relies on restating the governing equations to enable discontinuous space–time approximations of thermodynamic variables, and a variational continuous time integration. Numerical simulations of thermally unstable flows show the novel space–time formulation stably simulates mature turbulent dynamics over long time periods without any additional stabilisation, and appropriately conserves invariants. We further show how using Lagrange multipliers results in conservation of cubic invariants to machine precision. The inclusion of upwinded numerical fluxes is shown to suppress spurious oscillations while successfully conserving energy and monotonically damping entropy.

New twofold saddle-point formulations for poroelasticity with porosity-dependent permeability

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Collaborators: Bishnu P. Lamichhane and Ricardo Ruiz-Baier

We propose four-field and five-field Hu-Washizu-type mixed formulations for nonlinear poroelasticity, a coupled fluid diffusion and solid deformation process, considering that the permeability depends on a linear combination between fluid pressure and dilation. As the determination of the physical strains is necessary, the first formulation is written in terms of the primal unknowns of solid displacement and pore fluid pressure as well as the poroelastic stress and the infinitesimal strain, and it considers strongly symmetric Cauchy stresses. The second formulation imposes stress symmetry in a weak sense and it requires the additional unknown of solid rotation tensor. We study the unique solvability of the problem using the Banach fixed-point theory, properties of twofold saddle-point problems, and the Banach-Necas-Babuska theory. We propose monolithic Galerkin discretisations based on conforming Arnold-Winther for poroelastic stress and displacement, and either PEERS or Arnold-Falk-Winther finite element families for the stress-displacement-rotation field variables. The wellposedness of the discrete problem is established as well, and we show a priori error estimates in the natural norms. Some numerical examples are provided to confirm the rates of convergence predicted by the theory, and we also illustrate the use of the formulation in some typical tests in Biot poroelasticity.

Numerical analysis of a coupled thermoelastic–diffusion plate model

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Collaborators: Ricardo Ruiz-Baier and Neela Nataraj

We investigate the well-posedness of a coupled hyperbolic-parabolic system modeling diffusion in thermoelastic plates, consisting of a fourth-order hyperbolic PDE for the plate's deflection and second-order parabolic PDEs for the first moments of temperature and chemical potential. The unique solvability is established via Galerkin approach, and the additional regularity of the solution is also obtained under the appropriately strengthened given data. For numerical approximation, we employ the Newmark method for time discretization and a (C0-IP) scheme for the spatial discretization of displacement. For the first moments of temperature and chemical potential, we use the Crank-Nicolson method for time discretization and conforming finite elements for spatial discretization. The convergence of the fully discrete scheme with quasi-optimal rates in space and a quadratic rate in time is established. Several numerical examples are presented to validate the theoretical findings.

Convergence analysis of numerical approximations for total variation flow

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We perform numerical analysis for the regularised total variation flow using gradient discretisation method (GDM). GDM is an unified convergence analysis framework that covers conforming and non-conforming numerical methods, for instance, conforming and non-conforming $\mathbb{P}^1$ finite element, and two-point flux approximation. We propose a Gradient Scheme (GS), proved the existence and uniqueness of the solution to the GS, analyse stability and consistency of the GS, and establish the error estimates for the GS.

Numerical Optimisation

Organisers: Janosch Rieger, Lindon Roberts

* * *

First-order proximal splitting methods for distributed optimization

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Collaborators: Minh Dao and Matthew Tam

We consider finitely many agents over a connected network working cooperatively to solve a consensus optimisation problem. Each agent owns a private convex cost function with a decomposable structure given by the sum of two terms, one smooth and one non-smooth. In our decentralized setting, no agent has direct access to the information of the overall network, but instead they can only communicate with their neighbours in the network. We propose a primal-dual splitting method of proximal-gradient type with no central coordinator. Step-sizes are iteratively computed using backtracking line-search procedures and rounds of communication in the network. Our approach allows gradients to be only locally Lipschitz, relaxing the common assumption of L-smoothness without impairing convergence guarantees to minimisers.

New similarity-distance technique of intutionistic Fuzzy sets

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Collaborators: Duong Ton Dam

Intuitionistic fuzzy set (IFS), which is characterised by a degree of membership and a degree of nonmembership, is a very powerful tool to process vague information. After the pioneering study of Atanassov, the IFS has captured much attention from researchers in various fields, and many achievements have been made, such as the entropy measure of the IFS, the distance or similarity measure between IFSs, and the aggregation operators of the IFS. Specifically, this paper: Revisits certain existing similarity-distance techniques between IFSs; proposes an improved similarity-distance technique between IFSs. Applies the new similarity-distance technique to determine some decision-making situations.

A new local search algorithm for solving constrained DC optimisation

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Collaborators: Sona Taheri, Adil M. Bagirov, Andrew Eberhard

An optimisation algorithm is designed for solving constrained difference of convex (DC) programs. The sharp augmented Lagrangian approach is utilized to reformulate the constrained DC problem to unconstrained problem. Our proposed algorithm combines a local DC optimisation method with the well-known modified subgradient method, effectively extending the aggregate subgradient approach to address unconstrained DC optimisation problems. A detailed performance profile including comparison with some other existing constrained DC optimisation solvers is demonstrated to analyse the convergence of the stated method by applying the technique to numerous academic test problems.

A network model for urban planning based on a coupling between a Mean-Field Game and an optimal transportation problem

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Collaborators: Fabio Camilli and Luciano Marzufero

We present a mathematical model to describe the evolution of a city, which is determined by the interaction of two large populations of agents, workers, and firms. The map of the city is described by a network, with the edges representing at the same time residential areas and communication routes. The two populations compete for space while interacting through the labour market. The resulting model is described by a two-population mean-field game system coupled with an optimal transport problem. We prove the existence and uniqueness of the solution, and we provide several numerical simulations, discussing the numerical tools that we use.

Mixed precision in hierarchical basis finite element methods

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Collaborators: Linda Stals

The hierarchical multigrid algorithm, compared to the traditional multigrid method, is more suited for solving partial differential equations with complex boundaries and uneven solution distributions. The main difference between the both algorithms is that the traditional multigrid algorithm relies on geometric coarsening of regular physical grids, using restriction and interpolation to transition between grid layers for smoothing and refining the solution. In contrast, the hierarchical multigrid combines finite element method (FEM), smoothing based each level basis functions, with higher-level basis functions refining the result of lower-level basis functions, thus the hierarchical multigrid having a broader applicability. Nevertheless, hierarchical multigrid entails increased computational expense, particularly at finer levels. To address this, we propose enhancing the hierarchical multigrid algorithm via a mixed-precision computing framework: low-precision is used for coarser levels to accelerate global convergence, while high-precision is employed at finer levels to ensure solution accuracy. In this presentation, we will discuss the fundamental principles of the hierarchical multigrid method and and show how it improves accuracy over the multigrid algorithm. Finally, we will use numerical experiments to investigate the feasibility of mixed-precision acceleration in hierarchical multigrid.

Calculating minimum volume covering ellipsoids using leverage score sampling

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The Minimum Volume Covering Ellipsoid (MVCE) problem seeks to find the ellipsoid of minimum volume covering a set of n data points in d-dimensional Euclidean space. Although solution algorithms exist for the MVCE problem, computation times can be very expensive when n and d are large. Using leverage score sampling, we reduce the number of points considered by the algorithm, and hence speed up computation times. Additionally, under some conditions, we can prove that the computed solution is close to the exact solution.

Generalised Gearhart-Koshy acceleration is a Krylov space method

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Collaborators: Markus Hegland

The Gearhart-Koshy acceleration for the Kaczmarz method for linear systems is a line-search with the unusual property that it does not minimise the residual, but the error. This acceleration can be generalised from a line-search to a search in affine subspaces, which turns out to be a Krylov space method that minimises the Euclidean norm error over the Krylov space.

Faut tolerant multigrid

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Collaborators: Frederick Fung

The massive increase in the size and complexity of components in modern high-performance clusters has significantly reduced the mean time between failures. Traditional checkpoint-restart strategies have become too costly at exascale, leading algorithmic-based fault tolerance (ABFT) techniques to aid. These ABFT techniques have been applied to several popular numerical algorithms to provide algorithm-specific resilience against various types of faults. We study the resilience of the parallel multigrid algorithm defined on an adaptively refined mesh. Stals has demonstrated an algorithmic-based recovery approach that reconstructs the lost dynamic mesh data with as little redundancy as the coarsest grid. However, this still leaves the question of how to recover the local numerical data. The answer is not as straightforward as it may initially appear, as the local mesh stored in a processor may be non-nested with unaligned boundaries. We will present modifications to the multigrid iteration designed to reconstruct the lost numerical data as cheaply as possible.

A decentralised algorithm for min-max problems

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Collaborators: Mahadevan Ganesh and Stuart Hawkins

In this talk, we consider a connected network of finitely many agents working cooperatively to solve a min-max problem with convex-concave structure. We propose a decentralised first-order algorithm which can be viewed as combining features of two algorithms: PG-EXTRA for decentralised minimisation problems and the forward reflected backward method for (non- distributed) min-max problems. In each iteration of our algorithm, each agent computes the gradient of the smooth component of its local objective function as well as the proximal operator of its non-smooth component, following by a round of communication with its neighbours.

~~Coordinating a virtual power plant with a decentralised distributed algorithm~~

~~***Liam Timms****~~ (University of Melbourne)

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Collaborators: Matthew K. Tam and Joyce Zhang

Power banks present an increasingly accessible and adaptable way to use and store power. Multiple power banks can be coordinated to create a virtual power plant (VPP) that can satisfy larger power demands. However, coordinating a VPP introduces difficulties regarding how individual charging decisions interact. In this talk, we present a model for managing a VPP as a non-cooperative game with individual power banks as agents. To solve this model and find optimal charging schedules, we develop an algorithm based on monotone operator splitting. This algorithm is distributed to reflect the independent agents making up the VPP, and decentralised to avoid the drawbacks of a centrally coordinating agent.

Parallel level set-based optimisation of three-dimensional piezoelectric materials

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Collaborators: Anthony P. Roberts and Vivien J. Challis

Owing to their ability to generate voltage under deformation and vice versa, piezoelectric materials are utilised in several industrial applications including for sensing, actuating, and energy harvesting. Recent advancements of fine-scale additive manufacturing techniques have prompted the design of state-of-the-art heterogeneous piezoelectric meta-materials that exhibit exotic or enhanced properties. Optimisation of such materials can be achieved computationally using a mathematically motivated technique called topology optimisation. This is a class of PDE-constrained optimisation that seeks to minimise functionals that depend on the underlying domain and the solutions to PDE constraints. In this talk we will discuss computational techniques and results for memory-distributed topology optimisation of three-dimensional piezoelectric materials and structures using the level-set method. In the first part of the talk we will introduce parallel level set-based topology optimisation. Following this we will discuss homogenisation of periodic piezoelectric materials and consider preconditioning the coupled discretised linear system resulting from the finite element method. We use the developed techniques to design high-resolution piezoelectric meta-materials with enhanced properties that yield new insights into material design for sensing and hydrophone applications.

Interplay between machine learning and optimisation

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Collaborators: Lisa Chen and Tianyi Chen

Stochastic gradient methods (SGMs) have become the workhorse of machine learning (ML) due to their incremental nature with a computationally cheap update. In this talk, I will first discuss the close interaction between computational optimisation and statistical generalisation, a core concept in machine learning, for SGMs in the framework of statistical learning theory (SLT). The core concept for this study is algorithmic stability which characterises how the output of an ML algorithm changes upon a small perturbation of the training data. The first part will on the question of understanding the generalisation of over-parameterised neural networks trained by SGD. In the second part, I will briefly talk about the similar interaction arising in multi-objective optimisation and stochastic compositional optimisation algorithms.

Uncertainty Quantification and Stochastic PDEs

Organisers: Alexander Gilbert, Jörn Wichmann

* * *

On stochastic PDEs and their applications to derivative pricing through a conditional Feynman-Kac formula

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Collaborators: Ivan Guo, Gregoire Loeper

In a multi-dimensional diffusion framework, the price of a financial derivative can be expressed as an iterated conditional expectation, where the inner conditional expectation conditions on the future of an auxiliary process (usually volatility/variance) that enters into the dynamics for the spot. Inspired by results from non-linear filtering theory, we show that this inner conditional expectation solves a backward SPDE (a so-called 'conditional Feynman-Kac formula'), thereby establishing a connection between SPDE and derivative pricing theory. Through the conditional Feynman-Kac formula, we establish an alternative class of so-called mixed Monte-Carlo PDE numerical methods for pricing financial derivatives. We provide a simple demonstration of this method by pricing a European put option.

An efficient surrogate model for inversion of a class of wave configuration parameter

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Collaborators: Mahadevan Ganesh and Stuart Hawkins

We consider the inverse problem of determining the locations of multiple scatterers with known shape from noisy far field data. We use Bayesian inference, where the outcome is a posterior distribution of the possible scatterer locations. In practice, to extract information from the posterior requires a significant number of simulations of the forward model with a high-dimensional parameter space that includes the scatterer locations. We explore a surrogate model for the far field to substantially reduce computational time for the sampling-based simulations. Our novel, fast, and sufficiently accurate surrogate is based on principles of wave propagation and the structure of multiply-scattered waves.

A neural-network surrogate Bayesian algorithm for the Helmholtz inverse-shape problem

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Collaborators: Stuart C. Hawkins and Mahadevan Ganesh

We present a novel approach to the classical inverse problem of reconstructing the shape of scatterers from noisy far-field data. The far-field data in our model is generated by multiple incident waves striking an impenetrable scatterer. This data can be mathematically modeled using the Helmholtz equation in the unbounded region outside the scatterer. For reconstruction, our method employs a Bayesian framework that incorporates data and utilizes Markov Chain Monte Carlo (MCMC) sampling.

To address the computational challenges posed by the high-dimensional prior space, we introduce a physics-property informed (PPI) neural network (NN) surrogate model for the forward problem. The PPI component of the algorithm facilitates the training of the NN using far-field data from just one incident wave. Subsequently, the PPINN-surrogate model takes advantage of rotational symmetries in the prior space, allowing for efficient evaluation of the forward model across several incident wave directions. We showcase our method's effectiveness by demonstrating excellent reconstruction for a range of test scatterer shapes.

Function space embeddings and L_∞-approximation with infinitely many variables

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Collaborators: Michael Gnewuch (Osnabrück) and Klaus Ritter (Kaiserslautern)

We study a sequence of continuous approximation problems on function spaces $(\mathcal{H}_d)_{d\geq 1}$, where $d \geq 1$ denotes the number of variables the elements of $\mathcal{H}_d$ depend on; d is also called the dimension of the problem. In the field of Information-Based Complexity, one frequently studies approximation errors when d tends to infinity, and one tries to identify situations where a curse of dimensionality can be avoided.

It is known that certain sequences of function spaces $(\mathcal{H}_d)_{d\geq 1}$ with particular features facilitate the error analysis for certain types of algorithms. Embedding theorems for such sequences can help to transfer results from one sequence of function spaces to another. In the literature on this subject, reproducing kernel Hilbert spaces with tensor-product structure are frequently studied. In this talk we outline an approach to deal with embedding results that do not necessarily require the tensor-product structure, but allow for a more general setting. In particular, we are interested in L_∞ approximation in certain weighted function spaces with $d = \infty$, i.e., we consider an ∞-dimensional approximation problem.

Bayesian inference calibration of the modulus of elasticity

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Collaborators: Josef Dick, Kassem Mustapha (UNSW, Sydney)

This work uses the Bayesian inference technique to determine the Young modulus based on the linear elasticity equation with random Young modulus. The random Young modulus is approximated by a finite Karhunen–Loève expansion, while the solution to the linear elasticity equation is approximated by the finite element method. The high dimensional integral involving the posterior density and the quantity of interest is approximated by a higher-order quasi-Monte Carlo method.

Forecasting shipping freight rates and PDEs for their derivatives

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Collaborators: Changho Son

This presentation explores new findings related to shipping freight rates and methods for solving partial differential equations for derivatives based on these discoveries. According to S-H Lee (2023), despite the high volatility of shipping rates, their forecasting can be made with high accuracy using deep neural networks (DNN). This implies that the noise of the underlying asset may be colored noise, rather than white noise, at small time scales. Therefore, the author proposes that the underlying asset is governed by Brownian motion with a hidden Markov chain. Instead of relying on the Feynman-Kac formula, commonly used in previous studies, the author solves the partial differential equation directly. To achieve this, the perturbation method is applied, allowing the solution to be more easily understood through decomposition rather than approximation. Furthermore, this approach is flexible and can be readily extended to accommodate an increased number of regimes.

Doubling the convergence rate with kernel approximation

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Collaborators: Vesa Kaarnioja

This talk describes an approximation result, in joint work with Vesa Kaarnioja, where the proven convergence rate is twice that initially predicted. The application is to a kernel-based approximation (by Kaarnioja, Kazashi, Kuo, Nobile and Sloan) to the solution of a parametric partial differential equation.

Reaching the equilibrium: Long-term stable numerical schemes for SPDEs

Jörn Wichmann (Monash University)

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Collaborators: Kim-Ngan Le and Jérôme Droniou

Partial Differential Equations appear in many applications, such as modeling of fluids, porous media and superconductors, and are typically derived from physical principles. In extreme cases (e.g. at very fast or small scales), additional features need to be considered: Randomness takes into account model uncertainties that arise, for example, from thermal fluctuations and measurement errors. This motivates the use of SPDEs to improve the model's accuracy. In many cases, these models possess an energy structure, which characterises the stationary states of these systems. Unsteady solutions eventually tend to a steady state by dissipating their energy.

In this talk, we will explain how transport noise, a specific stochastic structure, enables full understanding of the energy dissipation of generalised Stokes' equations and how this relates to the stochastic steady state – an invariant measure. Moreover, we discuss how the energy dissipation can be preserved on the discrete level for a broad class of spatial discretisations. We conclude with numerical simulations.

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