

MCM 2025 DRAFT

Welcome to MCM 2025

We are delighted to welcome you to Chicago for the *16th International Conference on Monte Carlo and Quasi-Monte Carlo Methods in Scientific Computing*. The MCM conference series is, together with its sister conference series, the conferences on Monte Carlo Methods (MCM), a major event for researchers in the Monte Carlo and quasi-Monte Carlo community. We are glad to host MCM in Canada for a second time, the first being held in Montréal (2008).

MCM 2025 marks the thirty-year anniversary of the first MCM conference held in 1994. To celebrate this milestone, the organizing committee are excited to present a special panel session, followed by a Q&A. The panel members consist of Art Owen, Fred Hickernell, Frances Kuo, Alexander Keller and Josef Dick and the session will be moderated by Aretha Teckentrup. The motivation and purpose of this special event is to reflect on the past thirty years of progress in the field of MC and QMC methods and perhaps more importantly, to look ahead to what the big questions might reveal in the next thirty years and beyond.

As of July 5th, MCM 2024 features 137 talks, among them eight plenary talks, two tutorials, and twenty-four special sessions. The speakers come from a variety of scientific backgrounds, countries, institutions and stages of their career.

Located in South-West Ontario on the Grand River, Waterloo, or more widely known as part of the twin-cities of Kitchener-Waterloo (KW), offers cultural richness and technological innovation. Celebrated for its bustling tech scene, Waterloo has rightfully earned its part in the nickname "Silicon Valley North." In addition, KW boasts a rich cultural scene, highlighted by the annual Oktoberfest, the largest celebration of its kind outside of Germany. We hope that you enjoy what KW has to offer you away from campus!

We wish you a productive and interesting week at MCM 2024!

Fred Hickernell, Sou-Cheng Choi, Nathan Kirk, etc.
MCM 2025 Conference Organizers

Conference website: <https://ccbatiiit.github.io/mcm2025/>

Conference email: info@mcm2025chicago.org

Contents

MCM 2025 DRAFT	1
Welcome to MCM 2025	2
Contents	3
About MCM	4
History	4
Steering Committee	5
Scientific committee	6
Local Organizers	7
Local Technical and Support Team	7
Sponsors	7
Special Thanks	8
Schedule	9
Plenary Talks	21
Special Sessions	29
Abstracts	39
Special Session Talks	40
Contributed Talks	59
Practical Information	107
List of Participants	115

About MCM

History

The MCM Conference is a biennial meeting devoted to the study of Monte Carlo (MC) and quasi-Monte Carlo (QMC) methods, the relationships between the two classes of methods, and their effective application in different areas. Consistently attracting between one-hundred and two-hundred participants in recent years, its aim is to provide a forum where leading researchers and users can exchange information on the latest theoretical developments and important applications of these methods. The conference focuses primarily on the mathematical study of these techniques, their implementation and adaptation for concrete applications, and their empirical assessment.

The conference was initiated by Harald Niederreiter, who co-chaired the first seven conferences of the series. From 2006 onwards, the MCM Steering Committee has overseen the continuation of the conference series.

The previous instances of MCM were held in:

1. Las Vegas, USA (1994),
2. Salzburg, Austria (1996),
3. Claremont, USA (1998),
4. Hong Kong (2000),
5. Singapore (2002),
6. Juan-Les-Pins, France (2004),
7. Ulm, Germany (2006),
8. Montréal, Canada (2008),
9. Warsaw, Poland (2010),
10. Sydney, Australia (2012),
11. Leuven, Belgium (2014),
12. Stanford, USA (2016),
13. Rennes, France (2018),
14. Oxford, UK (2020, virtually),
15. Linz, Austria (2022).

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Capital
Markets

Special Thanks

The conference organizers would like to thank all sponsors for making this event possible. We also want to express our gratitude towards Professors Stefan Steiner and Changbao Wu (former and current Department Chair of Statistics and Actuarial Science at the University of Waterloo) and Professor Mark Giesbrecht (Dean, Faculty of Mathematics) for providing us with resources to help with the organization of this conference. We also thank the University of Waterloo for providing us with the space needed to host this conference.

We are also very grateful to our staff colleagues in the Department of Statistics and Actuarial Science for their unwavering assistance with many aspects of the organization, with special thanks in particular to Greg Preston, as well as Carla Daniels, Anthea Dunne, Carlos Mendes and Lucy Simpson.

We wish to extend our thanks to the entire Steering Committee and Scientific Program Committee, and past MCM conference organizers for their contribution and support. We also thank our plenary speakers, tutorial speakers, special session organizers, and all session chairs for their help and support with the scientific organisation of the conference. We are particularly grateful to Alex Keller, Frances Kuo, Peter Kritzer and Art Owen for providing detailed feedback and suggestions based on their past experience with the organization of the MCM conference.

Schedule

Mon, Jul 28	Session
08:00–17:30	Registration Desk Open
08:45–09:00	Conference Opening
09:00–10:00	Plenary Talk by Matt Pharr
10:00–10:30	Coffee Break
10:30–12:30	Track A: Stochastic Computation and Complexity, Part I
10:30–12:30	Track B: Domain UQ
10:30–12:30	Track C: Nested expectations: models and estimators, Part I
10:30–12:30	Track D: Hardware or Software for (Q)MC Algorithms, Part I
10:30–12:30	Track E: Technical Session 1 - MC
12:30–14:00	Lunch Break
14:00–15:00	Plenary Talk by Christiane Lemieux, U of Waterloo, Golden ratio nets and sequences
15:00–15:30	Coffee Break
15:30–17:30	Track F: Stochastic Computation and Complexity, Part II
15:30–17:30	Track G: Recent advances in Opt. under uncertainty
15:30–17:30	Track H: Comp. Methods for LD Sampl. and Appl.
15:30–17:30	Track I: Technical Session 4 - QMC, Part 1
15:30–17:30	Track J: Technical Session 12 - PDEs
17:30–19:30	Reception

Tue, Jul 29	Session
08:30–17:30	Registration Desk Open
09:00–10:00	Plenary Talk by Peter Glynn, Stanford U, Combining Sim. and Linear Algebra: COSIMLA
10:00–10:30	Coffee Break
10:30–12:30	Track A: Stochastic Computation and Complexity, Part III
10:30–12:30	Track B: Next-gen optimal Exp. Design: theory, scalability, and real world impact: Part I
10:30–12:30	Track C: Heavy-tailed Sampl.
10:30–12:30	Track D: Frontiers in (Q)MC and MC Methods, Part I
10:30–12:30	Track E: Technical Session 2 - Bayes Methods
12:30–14:00	Lunch Break
14:00–15:00	Plenary Talk by Roshan Joseph, Georgia Institute of Technology, Sensitivity and Screening: From MC to Exp. Design
15:00–15:30	Coffee Break
15:30–17:30	Track F: Stochastic Computation and Complexity, Part IV
15:30–17:30	Track G: Next-gen optimal Exp. Design: theory, scalability, and real world impact: Part II
15:30–17:30	Track H: Advances in Rare Events Sim.
15:30–17:30	Track I: Frontiers in (Q)MC and MC Methods, Part II
15:30–17:30	Track J: Technical Session 5 - QMC, Part 2

Wed, Jul 30	Session
08:30–16:30	Registration Desk Open
09:00–10:00	Plenary Talk by Michaela Szölgyenyi, U of Klagenfurt, An optimal transport approach to quantifying model uncertainty of SDEs
10:00–10:30	Coffee Break
10:30–12:30	Track A: Stochastic Computation and Complexity, Part V
10:30–12:30	Track B: Stat. DOE
10:30–12:30	Track C: Advances in Adaptive HMC
10:30–12:30	Track D: Technical Session 15 - Sim.
10:30–12:30	Track E: Technical Session 6 - Sampl.
12:30–14:00	Lunch Break
14:00–16:00	Track F: Stochastic Opt.
14:00–16:00	Track G: Recent Progress on Algorithmic Discr. Theory and Appl.
14:00–16:00	Track H: MC Appl. in HPC, Computer Graphics, and Computational Science
14:00–16:00	Track I: Technical Session 16 - Stat.
14:00–16:00	Track J: Technical Session 10 - Langevin
16:00–16:30	Coffee Break
18:00–20:30	Conference Dinner
Thu, Jul 31	Session
08:30–17:30	Registration Desk Open
09:00–10:00	Plenary Talk by Uros Seljak, UC Berkeley, Gradient-Based MCMC Sampl.: Methods and Opt. Strategies
10:00–10:30	Coffee Break
10:30–12:30	Track A: QMC and Appl. Part I
10:30–12:30	Track B: Anal. of Langevin and Related Sampl. Algorithms, Part I
10:30–12:30	Track C: Nested expectations: models and estimators, Part II
10:30–12:30	Track D: Technical Session 8 - Finance
10:30–12:30	Track E: Technical Session 13 - ML & Opt.
12:30–14:00	Lunch Break
14:00–15:00	Plenary Talk by Nicolas Chopin, Institut Polytechnique de Paris, Saddlepoint MC and its application to exact ecological inference
15:00–15:30	Coffee Break
15:30–17:30	Track F: QMC and Appl. Part II
15:30–17:30	Track G: Anal. of Langevin and Related Sampl. Algorithms, Part II
15:30–17:30	Track H: Recent Advances in Stochastic Gradient Descent
15:30–17:30	Track I: Technical Session 7 - Sampl.
15:30–17:30	Track J: Technical Session 11 - SDEs
18:00–20:30	Steering Committee Meeting (by invitation)
Fri, Aug 1	Session
08:30–12:15	Registration Desk Open
09:00–10:30	Track A: Forward and Inverse Problems for Stochastic Reaction Networks
09:00–10:30	Track B: Hardware or Software for (Q)MC Algorithms, Part II
09:00–10:30	Track C: Technical Session 3 - Sim.
09:00–10:30	Track D: Technical Session 9 - Sampl.
09:00–10:30	Track E: Technical Session 14 - MC
10:30–11	Coffee Break
11:00–12:00	Plenary Talk by Veronika Rockova
12:00–12:15	Closing Remarks

	Registration Desk Open			
	Conference Opening			
9:00 – 10:00	Plenary Talk: <i>Matt Phar</i> , p. ?? Chair:			
	Coffee Break			
	Special Session, TBD Stochastic Computation & Complexity, Part I, p. 30 Chair: <i>TBD</i>	Special Session, TBD Domain UQ, p. ?? Chair: <i>TBD</i>	Special Session, TBD Nested expectations: models & estimators, Part I, p. 31 Chair: <i>TBD</i>	Special Session, TBD Hardware or Software for (Q)MC Algorithms, Part I, p. ?? Chair: <i>TBD</i>
10:30–12:30	<i>Chengcheng Ling</i> , Quantitative approximation of stochastic kinetic equations: from discrete to continuum, p. 40	<i>André-Alexander Zepernick</i> , Domain UQ for stationary & time-dependent PDEs using QMC, p. ??	<i>Vesa Kaarnioja</i> , QMC for Bayes optimal Exp. Design with application to inverse problems governed by PDEs, p. 43	<i>Mike Giles</i> , CUDA implementation of MLMC on NVIDIA GPUs, p. ??
10:30–12:30	<i>Andreas Neuenkirch</i> , A strong order 1.5 boundary preserving discretization scheme for scalar SDEs defined in a domain, p. 41	<i>Carlos Jerez-Hanckes</i> , Domain UQ for Electromagnetic Wave Scattering via First- Order Sparse Boundary Element Approximation , p. ??	<i>Sebastian Krumscheid</i> , Double-loop RQMC estimator for nested integration, p. 44	<i>Pieterjan Robbe</i> , ML QMC without replications, p. ??
10:30–12:30	<i>Christopher Rauhögger</i> , An adaptive Milstein-type method for strong approximation of systems of SDEs with a discontinuous drift coefficient, p. 41	<i>Jürgen Dölz</i> , Quantifying uncertainty in spectral clusterings: expectations for perturbed & incomplete data, p. ??	<i>Vinh Hoang</i> , Posterior-Free A-Optimal Bayes DOE via Conditional Expectation, p. 44	<i>Irina-Beatrice Haas</i> , A nested ML MC framework for efficient simulations on FPGAs, p. ??
10:30–12:30	<i>Verena Schwarz</i> , Stong order 1 adaptive approximation of jump-diffusion SDEs with discontinuous drift, p. 42	<i>Harri Hakula</i> , Model Problems for PDEs on Uncertain Domains, p. ??		<i>Chung Ming Loi</i> , Scalable & User-friendly QMC Sampl. with UMBridge, p. ??
				<i>Zhihao Wang</i> , Stereographic Multi-Try Metropolis Algorithms for Heavy-tailed Sampl., p. 59
				<i>Ruben Seyer</i> , Creating rejection-free samplers by rebalancing skew-balanced jump processes, p. 60
				<i>Philippe Gagnon</i> , Theoretical guarantees for lifted samplers, p. 61

Jul 28, 2025 – Afternoon

Lunch Break					
14:00–15:00	Plenary Talk: <i>Christiane Lemieux, U of Waterloo, Golden ratio nets and sequences</i> , p. 22				Chair:
Coffee Break					
	Special Session, TBD Stochastic Computation & Complexity, Part II, p. 32 Chair: <i>TBD</i>	Special Session, TBD Recent advances in Opt. under uncertainty, p. ?? Chair: <i>TBD</i>	Special Session, TBD Comp. Methods for LD Sampl. & Appl., p. ?? Chair: <i>TBD</i>	TBD Tech. Sess. 4 - QMC, Part 1 Chair: <i>TBD</i>	TBD Tech. Sess. 12 - PDEs Chair: <i>TBD</i>
15:30–17:30	<i>Kateryna Pozharska</i> , Optimal designs for function discretization & construction of tight frames, p. 45	<i>Kateryna Pozharska</i> , Optimal designs for function discretization & construction of tight frames, p. ??	<i>Makram Chahine</i> , Improving Efficiency of Sampl.-based Motion Planning via Message-Passing MC, p. ??	<i>Christian Weiss</i> , Halton Sequences, Scrambling & the Inverse Star-Discrepancy, p. 69	<i>Adrien Richou</i> , A probabilistic Numerical method for semi-linear elliptic PDEs, p. 92
15:30–17:30	<i>Michael Gnewuch</i> , Optimality of deterministic & RQMC-cubatures on several scales of function spaces, p. 46	<i>Michael Gnewuch</i> , Optimality of deterministic & RQMC-cubatures on several scales of function spaces, p. ??	<i>Nathan Kirk</i> , Minimizing the Stein Discrepancy, p. ??	<i>Xiaoda Xu</i> , Star discrepancy & uniform approximation under weighted simple & stratified random Sampl., p. 69	<i>Abdujabar Rasulov</i> , MC method for the Spatially Homogenous Boltzmann equation, p. 92
15:30–17:30	<i>Leszek Plaskota</i> , Complexity of approximating piecewise smooth functions in the presence of deterministic or random noise, p. 47	<i>Leszek Plaskota</i> , Complexity of approximating piecewise smooth functions in the presence of deterministic or random noise, p. ??	<i>Gregory Seljak</i> , An Empirical Evaluation of Robust Estimators for RQMC, p. ??	<i>Sifan Liu</i> , Transport QMC, p. 70	<i>Miguel Alvarez</i> , A New Approach for Unbiased Estimation of Parameters of Partially Observed Diffusions, p. 93
15:30–17:30			<i>François Clément</i> , Searching Permutations for Constructing LD Point Sets & Investigating the Kritzing Sequence, p. ??	<i>Ambrose Emmett-Iwaniw</i> , Using Normalizing Flows for Efficient Quasi-Random Sampl. for Copulas, p. 70	<i>Håkon Hoel</i> , High-order adaptive methods for exit times of diffusion processes & reflected diffusions, p. 94
Reception					

Jul 29, 2025 – Morning

Registration Desk Open					
09:00–10:00	Plenary Talk: <i>Peter Glynn, Stanford U, Combining Sim. and Linear Algebra: COSIMLA</i> , p. 23 Chair:				
Coffee Break					
	Special Session, TBD Stochastic Computation & Complexity, Part III, p. 33 Chair: <i>TBD</i>	Special Session, TBD Next-gen optimal Exp. Design: theory, scalability, & real world impact: Part I, p. ?? Chair: <i>TBD</i>	Special Session, TBD Heavy-tailed Sampl., p. ?? Chair: <i>TBD</i>	Special Session, TBD Frontiers in (Q)MC & MC Methods, Part I, p. ?? Chair: <i>TBD</i>	TBD Tech. Sess. 2 - Bayes Methods Chair: <i>TBD</i>
10:30–12:30	<i>Sotirios Sabanis</i> , Wasserstein Convergence of Score-based Generative Models under Semiconvexity & Discontinuous Gradients, p. 47	<i>Ayoub Belhadji</i> , Weighted quantization using MMD: From mean field to mean shift via gradient flows, p. ??	<i>Sebastiano Grazi</i> , Parallel computations for Metropolis Markov chains Based on Picard maps, p. ??	<i>Sotirios Sabanis</i> , Wasserstein Convergence of Score-based Generative Models under Semiconvexity & Discontinuous Gradients, p. ??	<i>Lorenzo Nagar</i> , Optimizing Generalized Hamiltonian MC for Bayes Inference Appl., p. 62
10:30–12:30		<i>Adrien Corenflos</i> , A recursive MC approach to optimal Bayes Exp. Design, p. ??			<i>Hamza Ruzaygat</i> , Bayes Anomaly Detection in Variable-Order & Variable-Diffusivity Fractional Mediums, p. 63
10:30–12:30					<i>Arghya Datta</i> , Theoretical Guarantees of Mean Field Variational Inference for Bayes Principal Component Anal., p. 64
10:30–12:30					<i>Jimmy Lederman</i> , Bayes Anal. of Latent Underdispersion Using Discrete Order Stat., p. 64

Jul 29, 2025 – Afternoon

Lunch Break					
14:00–15:00	Plenary Talk: <i>Roshan Joseph, Georgia Institute of Technology, Sensitivity and Screening: From MC to Exp. Design</i> , p. 24 Chair: TBD				
Coffee Break					
	Special Session, TBD Stochastic Computation & Complexity, Part IV, p. 34 Chair: <i>TBD</i>	Special Session, TBD Next-gen optimal Exp. Design: theory, scalability, & real world impact: Part II, p. ?? Chair: <i>TBD</i>	Special Session, TBD Advances in Rare Events Sim., p. ?? Chair: <i>TBD</i>	Special Session, TBD Frontiers in (Q)MC & MC Methods, Part II, p. ?? Chair: <i>TBD</i>	TBD Tech. Sess. 5 - QMC, Part 2 Chair: <i>TBD</i>
15:30–17:30	<i>Larisa Yaroslavtseva</i> , Optimal strong approximation of SDEs with Hölder continuous drift coefficient, p. 48 <i>Alexander Steinicke</i> , Malliavin Differentiation of Lipschitz SDEs & BSDEs & an Application to Quadratic Forward-Backward SDEs, p. 49	<i>jacopo iollo</i> , Diffusion-Based Bayes Exp. Design: Advancing BED for Practical Appl., p. ?? <i>Alen Alexanderian</i> , Goal Oriented Sensor Placement for Infinite-Dimensional Bayes Inverse Problems, p. ??	<i>Bruno Tuffin</i> , Asymptotic robustness of smooth functions of rare-event estimators, p. ?? <i>Shyam Mohan Subbiah Pillai</i> , Estimating rare event probabilities associated with McKean–Vlasov SDEs, p. ??	<i>Takashi Goda</i> , Quasi-uniform QMC digital nets, p. ?? <i>Ziang Niu</i> , Boosting the inference for generative models by (Q)MC resampling, p. ??	<i>Peter Kritzer</i> , Approximation using median lattice algorithms, p. 71 <i>Yang Liu</i> , Convergence Rates of RQMC Methods under Various Regularity Conditions, p. 72
15:30–17:30	<i>Gunther Leobacher</i> , Tractability of L_2 -approximation & integration in weighted Hermite spaces of finite smoothness, p. 50	<i>Tommie Catanach</i> , Robust Bayes Optimal Exp. Design under Model Misspecification, p. ??	<i>Victor Elvira</i> , Multiple IS for Rare Event Sim. in Communication Systems, p. ??	<i>Chenyang Zhong</i> , A hit & run approach for Sampl. & analyzing ranking models, p. ??	<i>Jakob Dilen</i> , Use of rank-1 lattices in the Fourier neural operator, p. 73
15:30–17:30		<i>Xun Huan</i> , Optimal Pilot Sampl. for Multi-fidelity MC Methods, p. ??			<i>Aadit Jain</i> , Investigating the Optimum RQMC Batch Size for Betting & Empirical Bernstein Confidence Intervals, p. 73

Jul 30, 2025 – Morning

Registration Desk Open					
09:00–10:00	Plenary Talk: <i>Michaela Szölgényi, U of Klagenfurt, An optimal transport approach to quantifying model uncertainty of SDEs</i> , p. 25 Chair: TBD				
Coffee Break					
	Special Session, TBD Stochastic Computation & Complexity, Part V, p. 35 Chair: TBD	Special Session, TBD Stat. DOE, p. ?? Chair: TBD	Special Session, TBD Advances in Adaptive HMC, p. ?? Chair: TBD	TBD Tech. Sess. 15 - Sim. Chair: TBD	TBD Tech. Sess. 6 - Sampl. Chair: TBD
10:30–12:30	<i>Stefan Heinrich</i> , On the quantum complexity of parametric integration in Sobolev spaces, p. 50	<i>Simon Mak</i> , Respecting the boundaries: Space-filling designs for surrogate modeling with boundary information, p. ??	<i>Bob Carpenter</i> , GIST: Gibbs self-tuning for locally adapting Hamiltonian MC, p. ??	<i>Philippe Blondeel</i> , Combining QMC with Stochastic Optimal Control for Trajectory Opt. of Autonomous Vehicles in Mine Counter Measure Simulations, p. 100	<i>Akash Sharma</i> , Sampl. with constraints, p. 74
10:30–12:30	<i>Bernd Käßemodel</i> , Quantum Integration in Tensor Product Besov Spaces, p. 51	<i>Chaofan Huang</i> , Factor Importance Ranking & Selection using Total Indices, p. ??	<i>Nawaf Bou-Rabee</i> , Acceleration of the No-U-Turn Sampler, p. ??	<i>Rino Persiani</i> , A MC Approach to Designing a Novel Sample Holder for Enhanced UV-Vis Spectroscopy, p. 101	<i>Joonha Park</i> , Sampl. from high-dimensional, multimodal distributions using automatically tuned, tempered Hamiltonian MC, p. 75
10:30–12:30		<i>Chih-Li Sung</i> , Stacking designs: designing multi-fidelity computer experiments with target predictive accuracy, p. ??	<i>Trevor Campbell</i> , AutoStep: Locally adaptive involutive MCMC, p. ??	<i>Prasanth Shyamsundar</i> , ARCANEReweighting: A technique to tackle the sign problem in the Sim. of collider events in high energy physics, p. 102	<i>Arne Bouillon</i> , Localized consensus-based Sampl. for non-Gaussian distributions, p. 76
10:30–12:30			<i>Chirag Modi</i> , ATLAS: Adapting Trajectory Lengths & Step-Size for Hamiltonian MC, p. ??	<i>Nicole Aretz</i> , Multifidelity & Surrogate Modeling Approaches for UQ in Ice Sheet Simulations, p. 103	<i>Alex Shkolnik</i> , IS for Hawkes Processes, p. 76

Jul 30, 2025 – Afternoon

Lunch Break					
	Special Session, TBD Stochastic Opt., p. ?? Chair: <i>TBD</i>	Special Session, TBD Recent Progress on Algorithmic Discr. Theory & Appl., p. ?? Chair: <i>TBD</i>	Special Session, TBD MC Appl. in HPC, Computer Graphics, & Computational Science, p. ?? Chair: <i>TBD</i>	TBD Tech. Sess. 16 - Stat. Chair: <i>TBD</i>	TBD Tech. Sess. 10 - Langevin Chair: <i>TBD</i>
14:00–16:00	<i>Shane Henderson</i> , A New Convergence Anal. of Two Stochastic Frank-Wolfe Algorithms , p. ??	<i>Haotian Jiang</i> , Algorithmic Discr. Theory: An Overview, p. ??	<i>Stefan Heinrich</i> , On the quantum complexity of parametric integration in Sobolev spaces, p. ??	<i>Kazem Adeleke</i> , Empirical Stat. Comparative Anal. of SNP Heritability Estimators & Gradient Boosting Machines (GBM) Using Genetic Data from the UK Biobank, p. 103	<i>Atila Lovas</i> , Stochastic gradient Langevin dynamics with non-stationary data, p. 85
14:00–16:00	<i>Raghu Bollapragada</i> , MC Based Adaptive Sampl. Approaches for Stochastic Opt., p. ??	<i>Peng Zhang</i> , Improving the Design of Randomized Experiments via Discr. Theory, p. ??	<i>Bernd Käßemodel</i> , Quantum Integration in Tensor Product Besov Spaces, p. ??	<i>Carles Domingo-Enrich</i> , Cheap permutation testing, p. 104	<i>Iosif Lytras</i> , Sampl. with Langevin Dynamics from non-smooth & non-logconcave potentials., p. 86
14:00–16:00		<i>Aleksandar Nikolov</i> , Online Factorization for Online Discrepancy Minimization, p. ??		<i>Christopher Draper</i> , Moving PCG beyond LCGs, p. 105	<i>Sara Pérez-Vieites</i> , Langevin-based strategies for nested particle filters, p. 87
14:00–16:00				<i>Yiming Xu</i> , Hybrid least squares for learning functions from highly noisy data, p. 105	<i>Nikolaos Makras</i> , Taming the Interacting Particle Langevin Algorithm – The Superlinear Case, p. 88
Coffee Break Conference Dinner					

Jul 31, 2025 – Morning

Registration Desk Open					
09:00–10:00	Plenary Talk: <i>Uros Seljak, UC Berkeley, Gradient-Based MCMC Sampl.: Methods and Opt. Strategies</i> , p. 26 Chair:				
Coffee Break					
	Special Session, TBD QMC & Appl. Part I, p. ?? Chair: <i>TBD</i>	Special Session, TBD Anal. of Langevin & Related Sampl. Algorithms, Part I, p. ?? Chair: <i>TBD</i>	Special Session, TBD Nested expectations: models & estimators, Part II, p. 36 Chair: <i>TBD</i>	TBD Tech. Sess. 8 - Finance Chair: <i>TBD</i>	TBD Tech. Sess. 13 - ML & Opt. Chair: <i>TBD</i>
10:30–12:30	<i>Felix Bartel</i> , Exact discretization, tight frames & recovery via D-optimal designs, p. ??	<i>Lihan Wang</i> , Convergence rates of kinetic Langevin dynamics with weakly confining potentials, p. ??	<i>RAUL TEMPONE</i> , ML RQMC estimator for nested expectations, p. 52	<i>Matyokub Bakoev</i> , The SDEs of the Heston Model for Option Pricing, p. 80	<i>Frédéric Blondeel</i> , Learning cooling strategies in simulated annealing through binary interactions, p. 95
10:30–12:30	<i>Zhiqian He</i> , High-dimensional density estimation on unbounded domain, p. ??	<i>Peter Whalley</i> , Randomized Splitting Methods & Stochastic Gradient Algorithms, p. ??	<i>Matteo Raviola</i> , Stochastic gradient with least-squares control variates, p. 53	<i>Vincent Zhang</i> , Characterizing Efficacy of Geometric Brownian Motion Expectation-based Simulations on Low-Volatility American Common Stocks, p. 81	<i>Du Ouyang</i> , Accuracy of Discretely Sampled Stochastic Policies in Continuous-Time Reinforcement Learning, p. 95
10:30–12:30	<i>Mou Cai</i> , L2-approximation: using randomized lattice algorithms & QMC hyperinterpolation, p. ??	<i>Xiaoou Cheng</i> , Delocalization of Bias in Unadjusted Hamiltonian MC, p. ??	<i>Philipp Guth</i> , A one-shot method for Bayes optimal Exp. Design, p. 53	<i>Hao Quan</i> , Efficient Pricing for Variable Annuity via Sim., p. 83	<i>Wei Cai</i> , Martingale deep neural networks for quasi-linear PDEs & stochastic optimal controls in 10,000 dimensions, p. 96
10:30–12:30	<i>Frances Y. Kuo</i> , Application of QMC to Oncology, p. ??				<i>Yiqing Zhou</i> , Minimizing Functions with Sparse Samples: A Fast Interpolation Approach, p. 97

Jul 31, 2025 – Afternoon

Lunch Break					
14:00–15:00	Plenary Talk: <i>Nicolas Chopin, Institut Polytechnique de Paris, Saddlepoint MC and its application to exact ecological inference</i> , p. 28 Chair:				
Coffee Break					
	Special Session, TBD QMC & Appl. Part II, p. ?? Chair: <i>TBD</i>	Special Session, TBD Anal. of Langevin & Related Sampl. Algorithms, Part II, p. ?? Chair: <i>TBD</i>	Special Session, TBD Recent Advances in Stochastic Gradient Descent, p. 37 Chair: <i>TBD</i>	TBD Tech. Sess. 7 - Sampl. Chair: <i>TBD</i>	TBD Tech. Sess. 11 - SDEs Chair: <i>TBD</i>
15:30–17:30	<i>Kosuke Suzuki</i> , Quasi-uniform QMC lattice point sets, p. ??	<i>Krishnakumar Balasubramanian</i> , Finite-Particle Convergence Rates for Stein Variational Gradient Descent, p. ??	<i>Jose Blanchet</i> , Inference for Stochastic Gradient Descent with Infinite Variance, p. 54	<i>Kun-Lin Kuo</i> , Revisiting the Gibbs Sampler: A Conditional Modeling Perspective, p. 77	<i>Fabio Zoccolan</i> , Dynamical Low-Rank Approximation for SDEs: an interacting particle-system ROM, p. 88
15:30–17:30	<i>Zexin Pan</i> , QMC confidence intervals using quantiles of randomized nets, p. ??	<i>Yifan Chen</i> , Convergence of Unadjusted Langevin in High Dimensions: Delocalization of Bias, p. ??	<i>Jing Dong</i> , Stochastic Gradient Descent with Adaptive Data, p. 54	<i>Sascha Holl</i> , Concatenation of Markov processes for MC Integration, p. 77	<i>Riccardo Saporiti</i> , Comparing Probabilistic Load Forecasts: SDEs & Deep Learning, p. 90
15:30–17:30	<i>Dirk Nuyens</i> , Approximation of multivariate periodic functions, p. ??	<i>Molei Tao</i> , Langevin-Based Sampl. under Nonconvex Constraints, p. ??		<i>Josephine Westermann</i> , Polynomial approximation for efficient transport-based Sampl., p. 79	<i>Leon Wilkosz</i> , Forward Propagation of Low Discrepancy Through McKean–Vlasov Dynamics: From QMC to MLQMC, p. 91
15:30–17:30		<i>Stefan Oberdörster</i> , Accelerated Mixing of the No-U-turn Sampler, p. ??		<i>Souryadip Ghosh</i> , Fast Approximate Matrix Inversion via MCMC for Linear System Solvers, p. 79	
Steering Committee Meeting (by invitation)					

Aug 1, 2025 – Morning

Registration Desk Open				
	Special Session, TBD Forward & Inverse Problems for Stochastic Reaction Networks, p. 38 Chair: TBD	Special Session, TBD Hardware or Software for (Q)MC Algorithms, Part II, p. ?? Chair: TBD	TBD Tech. Sess. 3 - Sim. Chair: TBD	TBD Tech. Sess. 9 - Sampl. Chair: TBD
09:00–10:30	Maksim Chupin, Filtered Markovian Projection: Dimensionality Reduction in Filtering for Stochastic Reaction Networks, p. 55	Niklas Baumgarten, A High-performance Multi-level MC Software for Full Field Estimates & Appl. in Optimal Control, p. ??	Yashveer Kumar, MC Sim. approach to solve distributed order fractional Math. model, p. 66	Nicola Branchini, Revisiting self-normalized IS: new methods & diagnostics, p. 83 Kevin Bitterlich, Delayed Acceptance Slice Sampl.: A Two-Level method for Improved Efficiency in High-Dimensional Settings, p. 97
09:00–10:30	Zhou Fang, Fixed-budget Sim. method for growing cell populations, p. 56	Aleksei Sorokin, QMC Generators, Randomization Routines, & Fast Kernel Methods, p. ??	Serena Fattori, Benchmarking the Geant4-DNA 'UHDR' Example for MC Sim. of pH Effects on Radiolytic Species Yields Using a Mesoscopic Approach, p. 66	Daniel Yukimura, Quantitative results on Sampl. from quasi-stationary distributions, p. 84 Reuben Cohn-Gordon, Gradient-based MCMC in high dimensions, p. 98
09:00–10:30	Muruhan Rathinam, State & parameter inference in stochastic reaction networks, p. 57	Johannes Krotz, Hybrid MC methods for kinetic transport, p. ??	Toon Ingelaere, ML Sim. of ensemble Kalman methods: interactions across levels, p. 68	Amit Subrahmanya, Serial ensemble filtering with marginal coupling, p. 85 Philip Schaer, Parallel Affine Transformation Tuning: Drastically Improving the Effectiveness of Slice Sampl., p. 99
09:00–10:30	Sophia Münker, Dimensionality Reduction for Efficient Rare Event Estimation, p. 57		Muhammad Noor ul Amin, Adaptive Max-EWMA Control Chart with SVR: MC Sim. for Run Length Anal., p. 68	Annabelle Carrell, Low-Rank Thinning, p. 100
Coffee Break				
14:00 – 15:00	Plenary Talk: Veronica, p. ?? Chair:			
Closing Remarks				

Plenary Talks

Mon, Jul 28 14:00–15:00



Golden ratio nets and sequences

Christiane Lemieux

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Coauthor(s): Nathan Kirk and Jaspar Wiart

In this talk, we discuss nets and sequences constructed in an irrational base, focusing on the case of a base given by the golden ratio φ . We provide a complete framework to study equidistribution properties of nets in base φ , which among other things requires the introduction of a new concept of prime elementary intervals which differ from the standard definition used for integer bases. We define the one-dimensional van der Corput sequence in base φ and two-dimensional Hammersley point sets in base φ and we prove some properties for $(0, 1)$ -sequences and $(0, m, 2)$ -nets in base φ , respectively. This part of the talk is based on [1].

Building on this new framework, we propose an *interlaced Halton sequence* that makes use of integer *and* irrational-based van der Corput sequences and show empirically improved performance compared to the traditional Halton sequence [2]. In addition, we propose a scrambling algorithm for irrational-based digital sequences, which leverages dependence properties of scrambled digital nets [3].

- [1] N. Kirk, C. Lemieux and J. Wiart. Golden ratio nets and sequences. To appear in *Functiones and Approximatio*, 2025.
- [2] N. Kirk, C. Lemieux. An improved Halton sequence for implementation in quasi-Monte Carlo methods. *Proceedings of the 2024 Winter Simulation Conference*, 431–442, IEEE Press, Piscataway, NJ, 2024.
- [3] C. Lemieux and J. Wiart. On the distribution of scrambled $(0, m, s)$ -nets over unanchored boxes. In: *Monte Carlo and Quasi-Monte Carlo Methods 2020*, A. Keller (ed), Springer, 187–230, 2022.

Tue, Jul 29 09:00–10:00

**Combining Simulation and Linear Algebra: COSIMLA***Peter W. Glynn*

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Coauthor(s): Zeyu Zheng

In numerical computation for Markov chains and jump processes, matrix-based linear algebraic methods leverage fully the special structure of such models, allowing one to efficiently compute highly accurate solutions quickly. When the number of states is large or infinite, Monte Carlo simulation is an appealing alternative, typically allowing low accuracy solutions to be computed efficiently. In this talk, we describe COSIMLA, COmbined SIMulations and Linear Algebra. This new class of algorithms combines the best of the two numerical approaches, using matrix methods to compute expectations and probabilities in the truncated core of the state space, while one uses Monte Carlo to simulate path excursions outside the truncation. As a result, one can now compute high accuracy solutions for models with a very large state space. We show how the method applies to computing equilibrium quantities and various transient characteristics of Markov chains. These algorithms can typically be viewed as an application of conditional Monte Carlo. We also discuss how stratification can be conveniently applied in this setting to provide further variance reductions.

Tue, Jul 29 14:00–15:00



Sensitivity and Screening: From Monte Carlo to Experimental Design

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Identifying the most important factors affecting the output of a system from a set of potentially important factors is an important problem in scientific investigations. If a computational model is available to predict the output, we can use global sensitivity analysis to quantify the importance of each factor. There are many Monte Carlo-based methods available to estimate global sensitivity indices. However, their computation can become costly if the model is computationally expensive. In such cases, carefully designed experiments can be used for screening the factors. In this talk, I will explain some of these techniques and the latest developments, including their applications in active learning. I will also briefly explain how to estimate the sensitivity indices from noisy data when we do not know or have access to the model that generated the data.

- [1] Xiao, Q., Joseph, V. R., and Ray, D. M. (2023). *Maximum One-Factor-At-A-Time Designs for Screening in Computer Experiments*. *Technometrics*, 65, 220-230.
- [2] Song, D. and Joseph, V. R. (2025). *Efficient Active Learning Strategies for Computer Experiments*. <https://arxiv.org/abs/2501.13841>.
- [3] Huang, C. and Joseph, V. R. (2025). *Factor Importance Ranking and Selection using Total Indices*. *Technometrics*, <https://doi.org/10.1080/00401706.2025.2483531>.

Wed, Jul 30 09:00–10:00



An optimal transport approach to quantifying model uncertainty of SDEs

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Coauthor(s): Benjamin A. Robinson

A fundamental question in stochastic modelling is that of quantifying the effects of model uncertainty. In this context it is of interest to compute a distance between different stochastic models. A reasonable choice of distance is a modification of the Wasserstein distance on the space of probability measures called adapted Wasserstein distance, as it appears in bicausal optimal transport.

We solve constrained optimal transport problems in which the marginal laws are given by the laws of solutions of stochastic differential equations (SDEs). We consider SDEs with irregular coefficients, making only minimal regularity assumptions. Numerical methods are employed as a theoretical tool to bound the adapted Wasserstein distance. This opens the door for computing the adapted Wasserstein distance in a simple way. We show that this method can be applied to quantifying model uncertainty in stochastic optimisation problems.

Our approach successfully brings together optimal transport and numerical analysis of SDEs.

Thu, Jul 31 09:00–10:00



Gradient-Based MCMC Sampling: Methods and Optimization Strategies

Uroš Seljak

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Coauthor(s): Reuben Cohn-Gordon, Jakob Robnik

Gradient-based Markov Chain Monte Carlo (MCMC) methods significantly outperform gradient-free alternatives in sampling efficiency, particularly in high-dimensional spaces where they have become the standard approach. These methods leverage gradient information to guide the sampling process more intelligently than random-walk approaches. Two fundamental approaches that dominate this field are 1) Hamiltonian Monte Carlo (HMC), which employs principles from classical mechanics, treating the sampling problem as simulating Hamiltonian dynamics on an extended phase space. This approach naturally incorporates momentum variables that help the sampler traverse the parameter space more efficiently than simple random walks. 2) Langevin Monte Carlo (LMC), which utilizes stochastic differential equations that incorporate both gradient information and controlled noise injection. Recent theoretical developments have produced microcanonical versions of both Hamiltonian and Langevin samplers (MCHMC and MCLMC). These variants demonstrate measurably superior sampling efficiency compared to their canonical predecessors.

In addition to the choice of the method, practitioners face numerous algorithmic choices that can significantly impact performance: 1) Metropolis Adjustment: The decision whether to include Metropolis-Hastings correction steps involves trading exact preservation of the target distribution against computational speed. 2) Preconditioning: Incorporating problem-specific geometric information through preconditioning matrices can dramatically improve convergence rates, particularly for ill-conditioned target distributions. 3) Hyperparameter Tuning: Critical parameters include step sizes, trajectory lengths for HMC, and damping coefficients for Langevin methods. Recently, well tuned black-box methods have been developed that approach optimal performance. 4) Parallelization Strategy: parallel sampling on a GPU or CPU cluster enables dramatically reduced wall clock time to reach the required target accuracy. 5) Numerical Integration: Higher-order integrators can improve accuracy at the cost of additional gradient evaluations per step.

This goal of this talk is to provide guidance to the optimal choice among these methods, which depends on specific application requirements including computational budget, accuracy demands, and problem dimensionality. Understanding the theoretical trade-offs enables practitioners to select and configure samplers that best match their particular constraints and objectives.

Thu, Jul 31 14:00–15:00



Saddlepoint Monte Carlo and its Application to Exact Ecological Inference

Nicolas Chopin

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Coauthor(s): Théo Voldoire, Guillaume Rateau, Robin J. Ryder

In ecological inference, one wishes to model individual items, but perform inference based only on aggregate data. For instance, in two-round elections, we are interested the behaviour of individual voters, but only have access to aggregate vote numbers at each precinct. We develop an exact method for a large class of Ecological Inference Bayesian models, which scales to the large data setting. Our approach solves a more general problem: assuming X is a random vector and A a non-invertible matrix, one sometimes need to perform inference while only having access to samples of $Y = AX$. The corresponding likelihood is typically intractable. One may still be able to perform exact Bayesian inference using a pseudo-marginal sampler, but this requires an unbiased estimator of the intractable likelihood.

We propose saddlepoint Monte Carlo, a method for obtaining an unbiased estimate of the density of Y with very low variance, for any model belonging to an exponential family. Our method relies on importance sampling and characteristic functions, with insights brought by the standard saddlepoint approximation scheme with exponential tilting. We show that saddlepoint Monte Carlo makes it possible to perform exact inference on particularly challenging problems and datasets. We present a study of the carryover of votes between the two rounds of various French elections, using the finest available data (number of votes for each candidate in about 60,000 polling stations over most of the French territory).

We show that existing, popular approximate methods for ecological inference can lead to substantial bias; saddlepoint Monte Carlo is immune from this bias, and can handle ecological inference in the large data framework. We also present original results for the 2024 legislative elections on political centre-to-left and left-to-centre conversion rates when the far-right is present in the second round. Finally, we discuss other exciting applications for saddlepoint Monte Carlo in privacy and inverse problems, such as dealing with inference with empirical quantiles for continuous data.

- [1] Voldoire T., Chopin N., Rateau G. and Ryder R.J. (2024). Monte Carlo and its Application to Exact Ecological Inference, *arxiv 2410.18243*, <https://arxiv.org/abs/2410.18243>,

Special Sessions

Stochastic Computation and Complexity, Part I

Organizers:

Stefan Heinrich

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Session Description:

The session is devoted to algorithms and complexity for quadrature and strong approximation of SDEs and SPDEs, in particular under nonstandard assumptions, high and infinite dimensional integration and approximation, and stochastic optimization and neural networks, including connections to functional analysis and stochastic analysis.

Mon, Jul 28, 2025 – Morning, 10:30 – 12:30,

Chengcheng Ling

Quantitative Approximation of Stochastic Kinetic Equations: From Discrete to Continuum
p. 40

Andreas Neuenkirch

A Strong Order 1.5 Boundary Preserving Discretization Scheme for Scalar SDEs Defined in a Domain p. 41

Christopher Rauhögger

An Adaptive Milstein-Type Method for Strong Approximation of Systems of SDEs With a Discontinuous Drift Coefficient p. 41

Verena Schwarz

Strong Order 1 Adaptive Approximation of Jump-Diffusion SDEs With Discontinuous Drift
p. 42

Nested Expectations: Models and Estimators, Part I

Organizers:

*Arved Bartuska*King Abdullah University of Science and Technology and RWTH Aachen University
sarved.bartuska@kaust.edu.sa*Abdul-Lateef Haji-Ali*Heriot-Watt University
a.hajiali@hw.ac.uk**Session Description:**

Nested expectations arise in many applications, such as in engineering, mathematical finance, and medical decision-making. In addition to their nested structure, numerical estimations of such expectations are often complicated by singularities or discontinuities. Moreover, approximations when evaluating inner expectations using, for example, finite element or time-stepping schemes render traditional estimation methods such as double-loop Monte Carlo prohibitively expensive. This session will explore models and applications with this structure and methods for efficient estimation.

Mon, Jul 28, 2025 – Morning, 10:30 – 12:30,

*Vesa Kaarnioja*QMC for Bayesian Optimal Experimental Design With Application to Inverse Problems
Governed by PDEs p. 43*Sebastian Krumscheid*

Double-Loop Randomized Quasi-Monte Carlo Estimator for Nested Integration p. 44

Vinh Hoang

Posterior-Free A-Optimal Bayesian Design of Experiments via Conditional Expectation p. 44

Stochastic Computation and Complexity, Part II

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Session Description:

The session is devoted to algorithms and complexity for quadrature and strong approximation of SDEs and SPDEs, in particular under nonstandard assumptions, high and infinite dimensional integration and approximation, and stochastic optimization and neural networks, including connections to functional analysis and stochastic analysis.

Mon, Jul 28, 2025 – Afternoon, 15:30 – 17:30,

Kateryna Pozharska

Optimal Designs for Function Discretization and Construction of Tight Frames p. 45

Michael Gnewuch

Optimality of Deterministic and Randomized QMC-Cubatures on Several Scales of Function Spaces p. 46

Leszek Plaskota

Complexity of Approximating Piecewise Smooth Functions in the Presence of Deterministic or Random Noise p. 47

Stochastic Computation and Complexity, Part III

Organizers:

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Session Description:

The session is devoted to algorithms and complexity for quadrature and strong approximation of SDEs and SPDEs, in particular under nonstandard assumptions, high and infinite dimensional integration and approximation, and stochastic optimization and neural networks, including connections to functional analysis and stochastic analysis.

Tue, Jul 29, 2025 – Morning, 10:30 – 12:30,

Sotirios Sabanis

Wasserstein Convergence of Score-Based Generative Models Under Semiconvexity and Discontinuous Gradients p. 47

Stochastic Computation and Complexity, Part IV

Organizers:

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Session Description:

The session is devoted to algorithms and complexity for quadrature and strong approximation of SDEs and SPDEs, in particular under nonstandard assumptions, high and infinite dimensional integration and approximation, and stochastic optimization and neural networks, including connections to functional analysis and stochastic analysis.

Tue, Jul 29, 2025 – Afternoon, 15:30 – 17:30,

Larisa Yaroslavtseva

Optimal Strong Approximation of SDEs With Hölder Continuous Drift Coefficient p. 48

Alexander Steinicke

Malliavin Differentiation of Lipschitz SDEs and BSDEs and an Application to Quadratic Forward-Backward SDEs p. 49

Gunther Leobacher

Tractability of L_2 -Approximation and Integration in Weighted Hermite Spaces of Finite Smoothness p. 50

Stochastic Computation and Complexity, Part V

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Session Description:

The session is devoted to algorithms and complexity for quadrature and strong approximation of SDEs and SPDEs, in particular under nonstandard assumptions, high and infinite dimensional integration and approximation, and stochastic optimization and neural networks, including connections to functional analysis and stochastic analysis.

Wed, Jul 30, 2025 – Morning, 10:30 – 12:30,

Stefan Heinrich

On the Quantum Complexity of Parametric Integration in Sobolev Spaces p. 50

Bernd Kåßemodel

Quantum Integration in Tensor Product Besov Spaces p. 51

Nested Expectations: Models and Estimators, Part II

Organizer:

Session Description:

Arved Bartuska King Abdullah University of Science and Technology/RWTH Aachen University arved.bartuska@kust.edu.sa
 Lateef Haji-Ali Heriot-Watt University a.hajiali@hw.ac.uk
 Nested expectations arise in many applications, such as in engineering, mathematical finance, and medical decision-making. In addition to their nested structure, numerical estimations of such expectations are often complicated by singularities or discontinuities. Moreover, approximations when evaluating inner expectations using, for example, finite element or time-stepping schemes render traditional estimation methods such as double-loop Monte Carlo prohibitively expensive. This session will explore models and applications with this structure and methods for efficient estimation. List of speakers: Raúl Tempone (King Abdullah University of Science and Technology/RWTH Aachen University) André Gustavo Carlon (RWTH Aachen University) Zhijian He (South China University of Technology) Philipp Guth (Johann Radon Institute for Computational and Applied Mathematics)

Thu, Jul 31, 2025 – Morning, 10:30 – 12:30,

RAUL TEMPONE

Multilevel Randomized Quasi-Monte Carlo Estimator for Nested Expectations p. 52

Matteo Raviola

Stochastic Gradient With Least-Squares Control Variates p. 53

Philipp Guth

A One-Shot Method for Bayesian Optimal Experimental Design p. 53

Recent Advances in Stochastic Gradient Descent

Organizer:

Jing Dong

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Session Description:

Stochastic Gradient Descent (SGD) is a cornerstone optimization method in machine learning, renowned for its efficiency in handling large-scale data. Its iterative approach enables the processing of extensive datasets by updating model parameters using randomly selected data subsets, thereby reducing computational costs. Despite its widespread adoption, traditional SGD faces challenges such as convergence to sharp minima, and sensitivity to data distribution shifts. Addressing these challenges is crucial for enhancing model generalization, robustness, and overall performance in diverse applications. This session aims to delve into recent developments that address these challenges in SGD, presenting innovative methodologies and theoretical insights to enhance its effectiveness in complex learning scenarios. The session will have three to four speakers. Currently, the confirmed speakers are Jose Blanchet (Stanford University), Chang-Han Rhee (Northwestern University), and Jing Dong (Columbia University). Each will present their recent works on stochastic gradient descent, ranging from SGD and heavy-tailed phenomenon to SGD with adaptively generated data. Collectively, these talks will shed light on cutting-edge advancements in SGD methodologies, providing both theoretical frameworks and practical strategies to enhance optimization in complex, real-world applications.

Thu, Jul 31, 2025 – Afternoon, 15:30 – 17:30,

Jose Blanchet

Inference for Stochastic Gradient Descent With Infinite Variance p. 54

Jing Dong

Stochastic Gradient Descent With Adaptive Data p. 54

Forward and Inverse Problems for Stochastic Reaction Networks

Organizers:

Sophia Münker

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Session Description:

This session aims to bring together experts working on stochastic reaction networks and pure jump processes for modeling stochastic biological and chemical systems. The session is about recent advances in Monte Carlo methods, variance and dimension reduction techniques that are relevant for tackling forward and inverse problems. The speakers are:

- Zhou Fang (Academy of Mathematics and Systems Science, Chinese Academy of Sciences)
- Sophia Münker (RWTH Aachen University)
- Maksim Chupin (King Abdullah University of Science and Technology (KAUST))
- Muruhan Rathinam (University of Maryland Baltimore County)

Fri, Aug 1, 2025 – Morning, 09:00 – 10:30,

Maksim Chupin

Filtered Markovian Projection: Dimensionality Reduction in Filtering for Stochastic Reaction Networks p. 55

Zhou Fang

Fixed-Budget Simulation Method for Growing Cell Populations p. 56

Muruhan Rathinam

State and Parameter Inference in Stochastic Reaction Networks p. 57

Sophia Münker

Dimensionality Reduction for Efficient Rare Event Estimation p. 57

Abstracts

Special Session Talks

Mon, Jul 28 10:30–12:30

Quantitative Approximation of Stochastic Kinetic Equations: From Discrete to Continuum

Chengcheng Ling

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Coauthor(s): Stochastic Computation and Complexity, Part I

We study the strong convergence of a generic tamed Euler-Maruyama (EM) scheme for the kinetic type stochastic differential equation (SDE) (also known as second order SDE) driven by α -stable type noise with $\alpha \in (1, 2]$. We show that when the drift exhibits a relatively low regularity: anisotropic β -Hölder continuity with $\beta > 1 - \frac{\alpha}{2}$, the corresponding tamed EM converges with a convergence rate $(\frac{1}{2} + \frac{\beta}{\alpha(1+\alpha)} \wedge \frac{1}{2})$, which aligns with the results of first-order SDEs.

This talk is based on the work [arXiv:2409.05706](#) (joint with Zimo Hao and Khoa Lê) and the work [arXiv:2412.05142](#).

Mon, Jul 28 10:30–12:30

A strong order 1.5 boundary preserving discretization scheme for scalar SDEs defined in a domain*Andreas Neuenkirch*

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Coauthor(s): Ruishu Liu, Xiaojie Wang

Special session: Stochastic Computation and Complexity p.30

We study the strong approximation of scalar SDEs, which take values in a domain and have non-Lipschitz coefficients. By combining a Lamperti-type transformation with a semi-implicit discretization approach and a taming strategy, we construct a domain-preserving scheme that strongly converges under weak assumptions. Moreover, we show that this scheme has strong convergence order 1.5 under additional assumptions on the coefficients of the SDE. In our scheme, the domain preservation is a consequence of the semi-implicit discretization approach, while the taming strategy allows controlling terms of the scheme that admit singularities but are required to obtain the desired order.

Our general convergence results are applied to various SDEs from applications, with sub-linearly or super-linearly growing and non-globally Lipschitz coefficients.

- [1] Ruishu Liu, Andreas Neuenkirch and Xiaojie Wang (2024+). A strong order 1.5 boundary preserving discretization scheme for scalar SDEs defined in a domain. *Mathematics of Computation*. doi:10.1090/mcom/4014 (to appear, online first)

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Mon, Jul 28 10:30–12:30

Christopher Rauhögger*University of Passau*

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StochasticComputationandComplexity

We consider d -dimensional systems of SDEs with a discontinuous drift coefficient. More precisely, we assume that there exists a C^5 -hypersurface $\Theta \subseteq \mathbb{R}^d$ such that the drift coefficient is intrinsic Lipschitz continuous on $\mathbb{R}^d \setminus \Theta$ and has intrinsic Lipschitz continuous derivative on $\mathbb{R}^d \setminus \Theta$. Furthermore, the diffusion coefficient is C^1 on \mathbb{R}^d and commutative with a bounded derivative that is intrinsic Lipschitz continuous on $\mathbb{R}^d \setminus \Theta$.

It was proven in [1] for $d = 1$ and more recently in [2] for general $d \in \mathbb{N}$ that in this setting a transformed Milstein scheme achieves an L_p -error rate of order at least $3/4$ — in terms of the number of evaluations of the driving Brownian motion. Furthermore it was proven in

[3] that for $d = 1$ in the same setting an adaptive Milstein-type scheme achieves an L_p -error rate of order at least 1 in terms of the average number of evaluations of the driving Brownian motion.

In this talk we present a generalisation of the result from [3] to higher dimensions. More precisely, we introduce an adaptive transformed Milstein scheme which can be used for the approximation of solutions of d -dimensional systems of SDEs at the final time point in this setting and prove that this scheme achieves an L_p -error rate of order at least 1 in terms of the average number of evaluations of the driving Brownian motion.

- [1] M'uller-Gronbach, Thomas & Yaroslavtseva, Larisa. (2022). *A strong order 3/4 method for SDEs with discontinuous drift coefficient*. IMA Journal of Numerical Analysis. 42. 229-259
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- [3] Yaroslavtseva, Larisa. (2022). *An adaptive strong order 1 method for SDEs with discontinuous drift coefficient*. Journal of Mathematical Analysis and Applications. 513. 2. Paper Number 126180, 29

Mon, Jul 28 10:30–12:30

Strong order 1 adaptive approximation of jump-diffusion SDEs with discontinuous drift

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In this talk we present an adaptive approximation scheme for jump-diffusion SDEs with discontinuous drift and (possibly) degenerate diffusion. The scheme is a transformation-based doubly-adaptive quasi-Milstein scheme, which is doubly-adaptive in the sense that it is jump-adapted, i.e. all jump times of the Poisson noise are grid points, and it includes an adaptive stepsize strategy to account for the discontinuities of the drift. It is proven to have strong convergence rate 1 in L^p for $p \in [1, \infty)$ with respect to the average computational cost for these SDEs. To obtain our result, we prove that under slightly stronger assumptions which are still weaker than those in existing literature, a related doubly-adaptive quasi-Milstein scheme has convergence order 1.

Mon, Jul 28 10:30–12:30

QMC for Bayesian optimal experimental design with application to inverse problems governed by PDEs

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Coauthor(s): Claudia Schillings

Special session: Nested expectations: models and estimators, Part I p.31

The goal in Bayesian optimal experimental design (OED) is to maximize the expected information gain for the reconstruction of unknown quantities in an experiment by optimizing the placement of measurements. The objective function in the resulting optimization problem involves a multivariate double integral over the high-dimensional parameter and data domains. For the efficient approximation of these integrals, we consider a sparse tensor product combination of quasi-Monte Carlo (QMC) cubature rules over the parameter and data domains. For the parameterization of the unknown quantities, we consider a model recently studied by Chernov and Lê [1,2] as well as Harbrecht, Schmidlin, and Schwab [3] in which the input random field is assumed to belong to a Gevrey class. The Gevrey class contains functions that are infinitely many times continuously differentiable with a growth condition on the higher-order partial derivatives, but which are not analytic in general. Using the techniques developed in [4], we investigate efficient Bayesian OED for inverse problems governed by partial differential equations (PDEs).

- [1] Chernov, Alexey, & Lê, Tùng (2024). Analytic and Gevrey class regularity for parametric elliptic eigenvalue problems and applications. *SIAM Journal on Numerical Analysis*, **62**(4), 1874–1900.
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- [3] Harbrecht, Helmut, Schmidlin, Marc, & Schwab, Christoph (2024). The Gevrey class implicit mapping theorem with applications to UQ of semilinear elliptic PDEs. *Mathematical Models and Methods in Applied Sciences*, **34**(5), 881–917.
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Mon, Jul 28 10:30–12:30

Double-loop randomized quasi-Monte Carlo estimator for nested integration*Sebastian Krumscheid*

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Coauthor(s): Arved Bartuska, André Gustavo Carlon, Luis Espath, Raúl Tempone

We present a double-loop randomized quasi-Monte Carlo estimator for nested integrals. This estimator applies the randomized quasi-Monte Carlo (rQMC) method to both integrals in the nested setting. Error bounds are derived for outer integrands displaying singularities at the boundaries of the integration domain, based on Owen's work [1]. Standard error bounds via the Koksma–Hlawaka inequality are rendered ineffective as singularities lead to infinite Hardy–Krause variation. Moreover, finite element discretizations of the inner integrand are discussed, increasing the overall cost of nested integral estimators.

The effectiveness of the proposed estimator is demonstrated in the Bayesian design setting for the estimation of the expected information gain of an experiment. A truncation scheme of the observation noise present in the experiment model allows for the application of the derived error bounds. Applications from pharmacokinetics and thermomechanics demonstrate the efficiency of the proposed method in high dimensions.

- [1] Owen, Art B. (2006). *Halton sequences avoid the origin*. SIAM Review, 48:487–503.

Mon, Jul 28 10:30–12:30

Posterior-Free A-Optimal Bayesian Design of Experiments via Conditional Expectation*Truong Vinh Hoang*

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LuisEspath,SebastianKrumscheid,Ra\unhbox\voidb@x\bgroup\let\unhbox\voidb@x\setbox\@tempboxa\hbox{u\global\mathchardef\accent@spacefactor\spacefactor}\let\begin\group\let\typeout\protect\begin\group\def\MessageBreak{\Omega(Font)}\let\protect\immediate\write\m@ne{LaTeXFontInfo: oninputline164.}\end\group\end\group\relax\let\ignorespaces\relax\accent19u\egroup\spacefactor\accent@spacefactor\relaxTempone

We propose a novel approach for solving the A-optimal Bayesian design of experiments that does not require sampling or approximating the posterior distribution. In this setting, the objective function is the expected conditional variance (ECV). Our method estimates the ECV by leveraging conditional expectation, which we approximate using its orthogonal projection property. We derive an asymptotic error bound for this estimator and validate it through numerical experiments. The method is particularly efficient when the design param-

eter space is continuous. In such scenarios, the conditional expectation can be approximated non-locally using tools such as neural networks. To reduce the number of evaluations of the measurement model, we incorporate transfer learning and data augmentation. Numerical results show that our method significantly reduces model evaluations compared to standard importance sampling-based techniques. Code available at: <https://github.com/vinh-tr-hoang/DOEviaPACE>.

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<https://doi.org/10.1137/23M1603364>

Mon, Jul 28 15:30–17:30

Optimal designs for function discretization and construction of tight frames

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FelixBartel,LutzK\unhbox\voidb@x\bgroup\let\unhbox\voidb@x\setbox\@tempboxa\hbox{a\global\mathchardef\accent@spacefactor\spacefactor}\let\begin\group\let\typeout\protect\begin\group\def\MessageBreak{\Omega(Font)}\let\protect\immediate\write\m@ne{LaTeXFontInfo:oninputline195.}\endgroup\endgroup\relax\let\ignorespaces\relax\accent127a\egroup\spacefactor\accent@spacefactor\mmerer,MartinSch\unhbox\voidb@x\bgroup\let\unhbox\voidb@x\setbox\@tempboxa\hbox{a\global\mathchardef\accent@spacefactor\spacefactor}\let\begin\group\let\typeout\protect\begin\group\def\MessageBreak{\Omega(Font)}\let\protect\immediate\write\m@ne{LaTeXFontInfo:oninputline1}\endgroup\endgroup\relax\let\ignorespaces\relax\accent127a\egroup\spacefactor\accent@spacefactor\er,TinoUllrich

Coauthor(s): Stochastic Computation and Complexity

In the talk we will present a direct and constructive approach approach for the construction of tight frames and exact Marcinkiewicz-Zygmund inequalities in the Lebesgue space [1]. It is based on a similar procedure of maximization of the determinant of a certain Gramian matrix with respect to points and weights, already used in [2] for discretization problem for the uniform norm, and results in a discrete measure with at most $n^2 + 1$ atoms, which accurately subsamples the L_2 -norm of complex-valued functions contained in a given n -dimensional subspace.

This approach can as well be used for the reconstruction of functions from general RKHS in L_p where one only has access to the most important eigenfunctions. The general results apply to the d -sphere or multivariate trigonometric polynomials on \mathbb{T}^d spectrally supported on arbitrary finite index sets $I \subset \mathbb{Z}^d$. Numerical experiments indicate the sharpness of this result.

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Ullrich, Tino (2024). *Exact discretization, tight frames and recovery via D -optimal designs*. arXiv:2412.02489.

- [2] Krieg, David, & Pozharska, Kateryna, & Ullrich, Mario & Ullrich, Tino (2024). *Sampling projections in the uniform norm*. arXiv:2401.02220.

Mon, Jul 28 15:30–17:30

Optimality of deterministic and randomized QMC-cubatures on several scales of function spaces

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Special session: Stochastic Computation and Complexity p.32

We study the integration problem over the s -dimensional unit cube on four scales of Banach spaces of integrands. First we consider Haar wavelet spaces $H_{p,q,\alpha}$, $1 \leq p, q \leq \infty$, $\alpha > 1/p$, consisting of functions whose Haar wavelet coefficients exhibit a certain decay behavior measured by the parameters p, q , and, most importantly, α . We study the worst case error of a deterministic cubature rule over the norm unit ball and provide upper bounds for quasi-Monte Carlo (QMC) cubature rules based on arbitrary (t, m, s) -nets as well as matching lower error bounds for arbitrary cubature rules. These results show that using arbitrary (t, m, s) -nets as integration nodes yields the best possible rate of convergence. In the Hilbert space setting $p = 2 = q$ it was earlier shown by Heinrich, Hickernell and Yue [2] that scrambled (t, m, s) -nets yield optimal convergence rates in the randomized setting, where the randomized worst case error is considered.

We establish several suitable function space embeddings that allow to transfer the deterministic and randomized upper error bounds on Haar wavelet spaces to certain spaces of fractional smoothness $1/p < \alpha \leq 1$ and to Sobolev and Besov spaces of dominating mixed smoothness $1/p < a \leq 1$. Known lower bounds for Sobolev and Besov spaces of dominating mixed smoothness show that (deterministic or suitably randomized) (t, m, s) -nets yield optimal convergence rates also on the corresponding scales of spaces.

The talk is based on the preprint [1] and the master thesis of my student Yannick Meiners.

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Mon, Jul 28 15:30–17:30

Complexity of approximating piecewise smooth functions in the presence of deterministic or random noise*Leszek Plaskota*

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Coauthor(s): Stochastic Computation and Complexity

Consider the smoothness class of 1-periodic functions $f : \mathbb{R} \rightarrow \mathbb{R}$ for which

$$|f^{(r)}(x) - f^{(r)}(y)| \leq |x - y|^\rho, \quad x, y \in \mathbb{R},$$

where $r \in \{0, 1, 2, \dots\}$ and $0 < \rho \leq 1$. It is well known that the optimal worst case error of L^p -approximation ($1 \leq p \leq \infty$) of such functions that can be achieved from n exact evaluations of f is proportional to $e_n = n^{-(r+\rho)}$. Less obvious is what happens when the functions are piecewise smooth only with unknown break points. Even less obvious is the situation when the function values are additionally corrupted by some noise, i.e., when evaluating the value of f at x we obtain $y = f(x) + \xi$ where $|\xi| \leq \delta$ (deterministic noise) or ξ is a zero-mean random variable of variance σ^2 (random noise). In this talk we construct an algorithm which despite the presence of noise and break points achieves the worst case L^p -error still proportional to e_n provided the noise level δ or σ is of the same order e_n (except the case of $p = \infty$ and random noise where we have an additional logarithmic factor in the error). The algorithm uses divided differences and special adaptive extrapolation technique to locate the break points and approximate in their neighborhoods.

Tue, Jul 29 10:30–12:30

Wasserstein Convergence of Score-based Generative Models under Semiconvexity and Discontinuous Gradients*Sotirios Sabanis*

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Special session: Stochastic Computation and Complexity p.33

Score-based Generative Models (SGMs) approximate a data distribution by perturbing it with Gaussian noise and subsequently denoising it via a learned reverse diffusion process. These models excel at modeling complex data distributions and generating diverse sam-

ples, achieving state-of-the-art performance across domains such as computer vision, audio generation, reinforcement learning, and computational biology. Despite their empirical success, existing Wasserstein-2 convergence analysis typically assume strong regularity conditions—such as smoothness or strict log-concavity of the data distribution—that are rarely satisfied in practice.

In this work, we establish the first non-asymptotic Wasserstein-2 convergence guarantees for SGMs targeting semiconvex distributions with potentially discontinuous gradients. Our upper bounds are explicit and sharp in key parameters, achieving optimal dependence of $O(\sqrt{d})$ on the data dimension d and convergence rate of order one. The framework accommodates a wide class of practically relevant distributions, including symmetric modified half-normal distributions, Gaussian mixtures, double-well potentials, and elastic net potentials. By leveraging semiconvexity without requiring smoothness assumptions on the potential such as differentiability, our results substantially broaden the theoretical foundations of SGMs, bridging the gap between empirical success and rigorous guarantees in non-smooth, complex data regimes.

- [1] Bruno, Stefano & Sabanis, Sotirios (2025). *Wasserstein Convergence of Score-based Generative Models under Semiconvexity and Discontinuous Gradients*. ArXiv.

Tue, Jul 29 15:30–17:30

Optimal strong approximation of SDEs with Hölder continuous drift coefficient

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Coauthor(s): Simon Ellinger and Thomas Müller-Gronbach

We study strong approximation of the solution of a scalar stochastic differential equation (SDE)

$$\begin{aligned} dX_t &= \mu(X_t) dt + dW_t, \quad t \in [0, 1], \\ X_0 &= x_0 \end{aligned} \tag{5.1}$$

at the final time point 1 in the case that the drift coefficient μ is α -Hölder continuous with $\alpha \in (0, 1]$. Recently, it was shown in [1] that for such SDEs the equidistant Euler approximation achieves an L^p -error rate of at least $(1 + \alpha)/2$, up to an arbitrary small ε , in terms of the number of evaluations of the driving Brownian motion W . In this talk we present a matching lower error bound. More precisely, we show that the L^p -error rate $(1 + \alpha)/2$ can not be improved in general by no numerical method based on finitely many evaluations of W at fixed time points. For the proof of this result we choose μ to be the Weierstrass function and we employ the coupling of noise technique recently introduced in [2].

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stochastic sewing approach. Probab. Theory Related Fields, **181**(4), 975–1034

- [2] Müller-Gronbach, T. & Yaroslavl'tseva, L. (2023). Sharp lower error bounds for strong approximation of SDEs with discontinuous drift coefficient by coupling of noise. Ann. Appl. Probab. **33**, 902–935.

Tue, Jul 29 15:30–17:30

Malliavin differentiation of Lipschitz SDEs and BSDEs and an Application to Quadratic Forward-Backward SDEs

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Special session: Stochastic Computation and Complexity p.34

Geiss and Zhou [1] showed that SDEs and BSDEs with Lipschitz generators admit Malliavin differentiability in the Brownian setting. We extend and apply this result in the Lévy case and present a differentiation formula for coefficients that are Lipschitz in the solution variable with respect to the Skorohod metric. The obtained formula then allows us to show the existence and uniqueness of solutions to a class of quadratic and superquadratic forward-backward SDE systems.

- [1] Geiss, S. and Zhou, X. (2024). *Coupling of Stochastic Differential Equations on the Wiener Space*. <https://arxiv.org/pdf/2412.10836>.

Tue, Jul 29 15:30–17:30

Tractability of L_2 -approximation and integration in weighted Hermite spaces of finite smoothness

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Special session: Stochastic Computation and Complexity p.34

We consider integration and L_2 -approximation for functions over \mathbb{R}^s from weighted Hermite spaces as introduced in [1]. We study tractability of the integration and L_2 -approximation problem for the different Hermite spaces, which describes the growth rate of the information complexity when the error threshold ε tends to 0 and the problem dimension s grows to infinity. Our main results are characterizations of tractability in terms of the involved weights, which model the importance of the successive coordinate directions for functions from the weighted Hermite spaces.

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Wed, Jul 30 10:30–12:30

On the quantum complexity of parametric integration in Sobolev spaces

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Stochasticcomputationandcomplexity

We consider the following problem of parametric integration in Sobolev spaces. We seek to approximate

$$S : W_p^r(D) \rightarrow L_q(D_1), \quad (Sf)(s) = \int_{D_2} f(s, t) dt \quad (s \in D_1),$$

where

$$D = [0, 1]^d = D_1 \times D_2, \quad D_1 = [0, 1]^{d_1}, \quad D_2 = [0, 1]^{d_2},$$

$$1 \leq p, q \leq \infty, \quad d, d_1, d_2, r \in \mathbf{N}, \quad d = d_1 + d_2, \quad \frac{r}{d_1} > \left(\frac{1}{p} - \frac{1}{q} \right)_+.$$

We study the complexity of this problem in the quantum setting of Information-Based Complexity [1]. Under the assumption that $W_p^r(D)$ is embedded into $C(D)$ (embedding condition)

the case $p = q$ was solved by Wiegand [2]. Here we treat the case $p = q$ without embedding condition and the general case $p \neq q$ with or without the embedding condition. We also compare the rates with those in the (classical) randomized setting [3].

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Wed, Jul 30 10:30–12:30

Quantum Integration in Tensor Product Besov Spaces

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Special session: Stochastic Computation and Complexity p.35

We begin with a brief introduction to the basic concepts of quantum computing and quantum information-based complexity for multivariate integration and approximation problems in various smoothness classes. We then discuss characterizations of functions in tensor product Besov spaces (mixed smoothness) using the tensorized Faber-Cieselski basis with coefficients based on mixed iterated differences. Relying on such a decomposition we develop a quantum algorithm to establish bounds for the worst case quantum integration error for this function class.

Thu, Jul 31 10:30–12:30

Multilevel randomized quasi-Monte Carlo estimator for nested expectations*Raúl Tempone*

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Coauthor(s): Arved Bartuska, André Gustavo Carlon, Luis Espath, Sebastian Krumscheid

Estimation methods for nested integrals face several challenges, including nonlinearities separating the integrals, boundary singularities, and the need for numerical discretization of the integrand. In this talk, we present an advanced multilevel randomized double-loop quasi-Monte Carlo estimator that addresses these challenges by combining hierarchical approximations with deterministic and randomized quasi-Monte Carlo (rQMC) methods. This estimator is tailored towards scenarios where the inner integrand requires discretization via the finite element method and the outer integrand exhibits singularities at the boundaries of the integration domain.

Applications from Bayesian experimental design, in particular, the expected information gain (EIG) of an experiment, necessitate a truncation scheme for observation noise to rigorously bound the estimation error. This truncation affects the computational cost only by a logarithmic factor. Numerical experiments demonstrate the predicted optimal cost of almost $\mathcal{O}(TOL^{-1-\gamma/\eta_w})$ where γ and η_w signify the cost and weak rate of finite element discretizations, respectively.

Thu, Jul 31 10:30–12:30

Stochastic gradient with least-squares control variates*Matteo Raviola*

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Coauthor(s): Fabio Nobile, Nathan Schaeffer

The stochastic gradient (SG) method is a widely used approach for solving stochastic optimization problems, but its convergence is typically slow. Existing variance reduction techniques, such as SAGA [1], improve convergence by leveraging stored gradient information; however, they are restricted to settings where the objective functional is a finite sum, and their performance degrades when the number of terms in the sum is large. In this work, we propose a novel approach which also works when the objective is given by an expectation over random variables with a continuous probability distribution. Our method constructs a control variate by fitting a linear model to past gradient evaluations using weighted discrete least-squares, effectively reducing variance while preserving computational efficiency. We establish theoretical sublinear convergence guarantees and demonstrate the method's effectiveness through numerical experiments on random PDE-constrained optimization.

- [1] Defazio, A., Bach, F., & Lacoste-Julien, S. (2014). *SAGA: A fast incremental gradient method with support for non-strongly convex composite objectives*. Advances in neural information processing systems, 27.

Thu, Jul 31 10:30–12:30

A one-shot method for Bayesian optimal experimental design*Philipp A. Guth*

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Coauthor(s): Robert Gruhlke, Claudia Schillings

Special session: Nested expectations: models and estimators, Part II p.36

Bayesian optimal experimental design (BOED) problems often involve nested integrals, making their direct computation challenging. To address this, a one-shot optimization approach is proposed, which decouples the design parameters from the forward model during the optimization process. In addition, the solution of the forward model can be replaced by a surrogate that is trained during the one-shot optimization. This allows for the generation of computationally inexpensive samples. Efficient sampling strategies are particularly important in BOED, as they reduce the high computational cost of nested integration, ultimately making the optimization more tractable.

Thu, Jul 31 15:30–17:30

Inference for Stochastic Gradient Descent with Infinite Variance*Jose Blanchet*

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Special session: Recent Advances in Stochastic Gradient Descent p.37

Stochastic gradient descent (SGD) with infinite variance gradients arises, perhaps surprisingly, quite often in applications. Even in settings involving “finite variance” in theory, infinite variance models appear to provide a better statistical fit over spatial and temporal scales of interest in applied settings. Motivated by this, we investigate a general methodology that enables the development of valid confidence regions for SGD with infinite variance. Along the way, we also obtain key results and properties for SGD with infinite variance, for example, asymptotic limits, optimal convergence rates, etc., which are counterparts of celebrated results known only in the finite variance case.

Thu, Jul 31 15:30–17:30

Stochastic Gradient Descent with Adaptive Data*Jing Dong*

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Coauthor(s): Ethan Che, Xin Tong

Special session: Recent Advances in Stochastic Gradient Descent p.37

Stochastic gradient descent (SGD) is a powerful optimization technique that is particularly useful in online learning scenarios. Its convergence analysis is relatively well understood under the assumption that the data samples are independent and identically distributed (iid). However, applying SGD to policy optimization problems in operations research involves a distinct challenge: the policy changes the environment and thereby affects the data used to update the policy. The adaptively generated data stream involves samples that are non-stationary, no longer independent from each other, and affected by previous decisions. The influence of previous decisions on the data generated introduces bias in the gradient estimate,

which presents a potential source of instability for online learning not present in the iid case. In this paper, we introduce simple criteria for the adaptively generated data stream to guarantee the convergence of SGD. We show that the convergence speed of SGD with adaptive data is largely similar to the classical iid setting, as long as the mixing time of the policy-induced dynamics is factored in. Our Lyapunov-function analysis allows one to translate existing stability analysis of stochastic systems studied in operations research into convergence rates for SGD, and we demonstrate this for queueing and inventory management problems. We also showcase how our result can be applied to study the sample complexity of an actor-critic policy gradient algorithm.

Fri, Aug 1 09:00–10:30

Filtered Markovian Projection: Dimensionality Reduction in Filtering for Stochastic Reaction Networks

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Special session: Forward and Inverse Problems for Stochastic Reaction Networks p.38

Stochastic reaction networks (SRNs) model stochastic effects for various applications, including intracellular chemical or biological processes and epidemiology. A key challenge in practical problems modeled by SRNs is that only a few state variables can be dynamically observed. Given the measurement trajectories, one can estimate the conditional probability distribution of unobserved (hidden) state variables by solving a system filtering equation. The current numerical methods, such as the Filtered Finite State Projection [1], are hindered by the curse of dimensionality, significantly affecting their computational performance. To overcome this, we propose to use a dimensionality reduction technique based on the Markovian projection (MP), initially introduced for forward problems [2]. In this work, we explore how to adapt the existing MP approach to the filtering problem and introduce a novel version of the MP, the Filtered MP, that guarantees the consistency of the resulting estimator [3]. The novel method employs a reduced-variance particle filter for estimating the jump intensities of the projected model and solves the filtering equations in a low-dimensional space, improving computational efficiency over existing methods.

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Fri, Aug 1 09:00–10:30

Fixed-budget simulation method for growing cell populations

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Special session: Forward and Inverse Problems for Stochastic Reaction Networks p.38

Investigating the dynamics of growing cell populations is crucial for unraveling key biological mechanisms in living organisms, with many important applications in therapeutics and biochemical engineering. Classical agent-based simulation algorithms are often inefficient for these systems because they track each individual cell, making them impractical for fast (or even exponentially) growing cell populations. To address this challenge, we introduce a novel stochastic simulation approach based on a Feynman-Kac-like representation of the population dynamics. This method, named the Feynman-Kac-inspired Gillespie's Stochastic Simulation Algorithm (FKG-SSA), always employs a fixed number of independently simulated cells for Monte Carlo computation of the system, resulting in a constant computational complexity regardless of the population size. Furthermore, we theoretically show the statistical consistency of the proposed method, indicating its accuracy and reliability. Finally, a couple of biologically relevant numerical examples are presented to illustrate the approach. Overall, the proposed FKG-SSA effectively addresses the challenge of simulating growing cell populations, providing a solid foundation for better analysis of these systems.

Fri, Aug 1 09:00–10:30

State and parameter inference in stochastic reaction networks*Muruhan Rathinam*

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Continuous time Markov chain models are widely used to model intracellular chemical reactions networks that arise in systems and synthetic biology. In this talk, we address the problem of inference of state and parameters of such systems from partial observations. We present details of recent particle filtering methods that are applicable to two different scenarios: one in which the observations are made continuously in time and the other in which the observations are made in discrete snapshots of time. We provide the theoretical justification as well as numerical results to illustrate these methods.

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Fri, Aug 1 09:00–10:30

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Coauthor(s): Forward and Inverse Problems for Stochastic Reaction Networks

A Stochastic Reaction Network (SRN) is a continuous-time, discrete-space Markov chain that models the random interaction of d species through reactions, commonly applied in biochemical systems. We are interested in efficiently estimating rare event probabilities, where we consider path-dependent observables. Therefore, we present an importance sampling (IS) method based on the discrete Tau-Leap (TL) scheme to enhance the performance of Monte Carlo (MC) estimators. The primary challenge in IS is selecting an appropriate change of probability measure to significantly reduce variance, which often requires deep insights into the underlying problem. To address this, we propose a generic approach to obtain an efficient path-dependent measure change, based on an original connection between finding optimal IS parameters and solving a variance minimization problem using a stochastic optimal control

(SOC) formulation [1]. The optimal IS parameters can be derived by solving a Hamilton-Jacobi-Bellman equation.

To address the curse of dimensionality, we propose the Markovian Projection (MP) technique to reduce the SRN to a lower-dimensional SRN (called MP-SRN) while preserving the marginal distribution of the original high-dimensional system. When solving the resulting SOC problem numerically to derive the variance reducing IS parameters, we derive the parameter for a reduced-dimensional model. These IS parameters can be applied to the full-dimensional SRN in the forward run. Analysis and numerical experiments demonstrate that our IS strategies substantially reduce the variance of the MC estimator, leading to lower computational complexity in the rare event regime compared to standard MC methods.

At the end of the talk, we give a small outlook on a multilevel-IS scheme to further improve the efficiency of the estimator.

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Contributed Talks

Mon, Jul 28 10:30-12:30

Stereographic Multi-Try Metropolis Algorithms for Heavy-tailed Sampling

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We introduce a novel family of gradient-free Markov chain Monte Carlo (MCMC) algorithms that integrate the principles of multi-try Metropolis (MTM) and stereographic MCMC, designed specifically for efficient sampling of heavy-tailed distributions. Through scaling analysis and extensive simulations, we demonstrate that the proposed stereographic multi-try Metropolis (SMTM) algorithm outperforms both traditional Euclidean MTM and existing stereographic random-walk Metropolis. Furthermore, the SMTM algorithm has the potential to benefit from modern hardware, such as GPUs, allowing for improved performance through parallel implementation.

Mon, Jul 28 10:30-12:30

Creating rejection-free samplers by rebalancing skew-balanced jump processes*Ruben Seyer*

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Coauthor(s): Erik Jansson, Moritz Schauer, Akash Sharma

Markov chain sampling methods form the backbone of modern computational statistics. However, many popular methods are prone to random walk behaviour, i.e. diffusion-like exploration of the sample space, leading to slow mixing that requires intricate tuning to alleviate. Non-reversible samplers can resolve some of these issues. We introduce a device that turns jump processes that satisfy a skew-detailed balance condition for a reference measure into a process that samples a target measure that is absolutely continuous with respect to the reference measure. This sampler is rejection-free, non-reversible and time-continuous. As an example, we apply the device to Hamiltonian dynamics discretized by the leapfrog integrator, resulting in a rejection-free non-reversible time-continuous version of Hamiltonian Monte Carlo (HMC). We prove the geometric ergodicity of the resulting sampler, and demonstrate its increased robustness to hyperparameter tuning compared to HMC through numerical examples. This comes at a computational cost at worst double that of HMC, in practice lower than other popular non-reversible samplers such as the Bouncy Particle Sampler.

Mon, Jul 28 10:30-12:30

Theoretical guarantees for lifted samplers*Philippe Gagnon*

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The work I would like to present is about a particular class of Markov chain Monte Carlo (MCMC) methods which use non-reversible Markov chains commonly referred to as *lifted Markov chains*; the methods are commonly referred to as *lifted samplers*. The methods are not particularly new (they date back at least to Horowitz [1]), but they have recently been the subject of significant research work motivated by a general belief that, in statistical applications, they lead to more efficient estimators than their reversible counterparts which correspond to Metropolis–Hastings (MH) algorithms (see, e.g., Andrieu and Livingstone [2]). It was thus somewhat surprising to observe that it is not always the case in some recent work (see, e.g., Gagnon and Maire [3]). One can thus wonder what degree of inefficiency these chains may exhibit in worst-case scenarios. This is an important question given that lifted samplers are popular in practice, a consequence of the fact that they are often as easy to implement on a computer as their MH counterparts and often have the same computational complexity.

The main contribution of our work is to provide an answer to this question under arguably the most general framework. We proceed by leveraging the seminal work of Tierney [4] to define a lifted version of a generalized MH algorithm. Virtually any (reversible) MCMC method can be seen as a special case of this generalized MH algorithm, ranging from the traditional MH algorithm of Hastings [5] to the reversible jump algorithm of Green [6]. Our main theoretical result allows for a comparison between the generalized MH algorithm and its lifted version in terms of the variance of produced estimators. It essentially guarantees that the variance of estimators produced by the lifted version cannot be more than twice that of estimators produced by the generalized MH algorithm. This result indicates that, while there is potentially a lot to gain from lifting a Markov chain, there is not much to lose. We also show that our result is optimal, in the sense that it is not possible to improve on the factor 2 without additional assumptions. The definition of the lifted version of the generalized MH algorithm allows to understand how a lifted sampler can be constructed under such a general framework, which adds a methodological contribution to our theoretical contribution.

The efficiency of Markov chains is traditionally assessed by studying the characteristics of their Markov transition operators. To establish our theoretical result, we needed to connect the efficiency of two significantly different operators (those of the MH and lifted algorithms): in addition to not be defined on the same domain, one is self-adjoint while the other is not, which further complicates the analysis. One of our main achievements was to identify a specific auxiliary operator which acts a bridge and allows to connect the efficiency of the two aforementioned operators. This auxiliary operator is compared to the MH one through a Peskun ordering [7] established via a careful analysis of the Markov kernels, yielding sharp bounds. The connections between the MH and lifted algorithms is completed by comparing the auxiliary operator with the lifted one using a result in Andrieu and Livingstone [2].

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Tue, Jul 29 10:30-12:30

Optimizing Generalized Hamiltonian Monte Carlo for Bayesian Inference applications

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In contrast to the widely adopted Hamiltonian/Hybrid Monte Carlo (HMC) [1], the Generalized Hamiltonian Monte Carlo (GHMC) algorithm [2, 3] leverages the irreversibility of its generated Markov chains, resulting in faster convergence to equilibrium and reduced asymptotic variance [4, 5].

Despite its theoretically predicted advantages, GHMC can be highly sensitive to the choice of a numerical integrator for the Hamiltonian equations and requires careful tuning of simulation parameters, such as the integration step size, the trajectory length, and the amount of random noise in momentum refreshment.

In this talk, we present a novel approach for finding optimal (in terms of sampling performance and accuracy) settings for a GHMC simulation. For an arbitrary simulated system, our methodology identifies a system-specific integration scheme that maximizes a conservation of energy for harmonic forces, along with appropriate randomization intervals for the simulation parameters, without incurring additional computational cost.

Numerical experiments on well-established statistical models exhibit, with the help of the state-of-the-art performance metrics, significant gains in GHMC sampling efficiency when

optimally tuned hyperparameters are chosen instead of heuristic or recommended ones. Comparative performance of GHMC and HMC with optimal settings is also discussed.

Additionally, we apply our methodology to three real-world case studies:

- Patient resistance to endocrine therapy in breast cancer;
- Influenza A (H1N1) epidemics outbreak;
- Modeling of cell-cell adhesion dynamics.

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Tue, Jul 29 10:30-12:30

Bayesian Anomaly Detection in Variable-Order and Variable-Diffusivity Fractional Mediums

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Fractional diffusion equations (FDEs) are powerful tools for modeling anomalous diffusion in complex systems, such as fractured media and biological processes, where nonlocal dynamics and spatial heterogeneity are prominent. These equations provide a more accurate representation of such systems compared to classical models but pose significant computational challenges, particularly for spatially varying diffusivity and fractional orders. In this talk I will present a Bayesian inverse problem for FDEs in a 2-dimensional bounded domain with an anomaly of unknown geometric and physical properties, where the latter are the diffusivity and fractional order fields. To tackle the computational burden of solving dense and ill-conditioned systems, we employ an advanced finite-element scheme incorporating low-rank

matrix representations and hierarchical matrices. For parameter estimation, we implement two surrogate-based approaches using polynomial chaos expansions: one constructs a 7-dimensional surrogate for simultaneous inference of geometrical and physical parameters, while the other leverages solution singularities to separately infer geometric features, then constructing a 2-dimensional surrogate to learn the physical parameters and hence reducing the computational cost immensely. These surrogates are used inside a Markov chain Monte Carlo algorithm to infer the unknown parameters.

Tue, Jul 29 10:30-12:30

Theoretical Guarantees of Mean Field Variational Inference for Bayesian Principal Component Analysis

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In this talk, we will investigate mean field variational inference for Bayesian principal component analysis (BPCA). Despite the wide usage of mean field variational inference for the BPCA model, there exists remarkably little theoretical justification. I will talk about new results on the convergence guarantees of the iterative coordinate ascent variational inference (CAVI) algorithm for the BPCA model. In particular, we will show that under reasonable technical assumptions on the initialization, CAVI converges exponentially fast to a local optimum. An interesting connection between the CAVI algorithm for the BPCA model and power iteration, which is a popular iterative numerical algorithm for finding singular vectors of a given matrix, will also be discussed.

Tue, Jul 29 10:30-12:30

Bayesian Analysis of Latent Underdispersion Using Discrete Order Statistics

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Researchers routinely analyze count data using models based on a Poisson likelihood, for which there exist many analytically convenient and computationally efficient strategies for

posterior inference. A limitation of such models however is the equidispersion constraint of the Poisson distribution. This restriction prevents the model’s likelihood, and by extension its posterior predictive distribution, from concentrating around its mode. As a result, these models are parametrically bound to produce probabilistic predictions with high uncertainty, even in cases where low uncertainty is supported by the data. While count data often exhibits overdispersion *marginally*, such data may nevertheless be consistent with a likelihood that is underdispersed *conditionally*, given parameters and latent variables. Detecting conditional underdispersion, however, requires one to fit the “right” model and thus the ability to build, fit, and critique a variety of different models with underdispersed likelihoods. Towards this end, we introduce a novel family of models for conditionally underdispersed count data whose likelihoods are based on order statistics of Poisson random variables. More specifically, we assume that each observed count coincides with the j^{th} order-statistic of D latent i.i.d. Poisson random variables, where j and D are user-defined hyperparameters. To perform efficient MCMC-based posterior inference in this family of models, we derive a data-augmentation strategy which samples the other $D-1$ latent variables from their exact conditional, given the observed (j, D) -order statistic. By relying on the explicit construction of a Poisson order statistic, this data augmentation strategy can be modularly combined with the many existing inference strategies for Poisson-based models. We generalize this approach beyond the Poisson to any non-negative discrete parent distribution and, in particular, show that models based on negative binomial order statistics can flexibly capture both conditional under and overdispersion. To illustrate our approach empirically, we build and fit models to three real count data sets of flight times, COVID-19 cases counts, and RNA-sequence data, and we demonstrate how models with underdispersed likelihoods can leverage latent structure to make more precise probabilistic predictions. Although the possibility of conditional underdispersion is often overlooked in practice, we argue that this is at least in part due to the lack of tools for modeling underdispersion in settings where complex latent structure is present.

Fri, Aug 1 09:00–10:30

Monte Carlo simulation approach to solve distributed order fractional mathematical model

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This work presents a novel approach to solving time-distributed order fractional nonhomogeneous differential equations using the Monte Carlo simulation method. Fractional differential equations with distributed orders are critical for modeling complex systems with memory and hereditary effects, such as viscoelastic materials, anomalous diffusion, and biological processes. The inclusion of time-distributed orders introduces additional challenges in analytical and numerical solutions, especially in the presence of nonhomogeneous terms.

The proposed Monte Carlo method reformulates the distributed order fractional equation into an equivalent integral representation. By simulating random processes and utilizing probabilistic interpretations of fractional operators, the solution is computed as a average over numerous realizations. The flexibility of Monte Carlo simulations makes them particularly well-suited for addressing the inherent complexity of distributed order systems.

Numerical experiments validate the efficiency and effectiveness of the Monte Carlo approach, illustrating its capability to handle various distributed order kernels and nonhomogeneous terms. This method offers a robust, scalable, and versatile framework for solving fractional differential equations, paving the way for broader applications in science and engineering.

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- [3] Kumar, Yashveer & Singh, Vineet Kumar (2021). *Computational approach based on wavelets for financial mathematical model governed by distributed order time-fractional partial differential equation*. Mathematics and Computers in Simulation, 190, 531-569.

Fri, Aug 1 09:00–10:30

Benchmarking the Geant4-DNA 'UHDR' Example for Monte Carlo Simulation of pH Effects on Radiolytic Species Yields Using a Mesoscopic Approach

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Background and Aims

FLASH radiotherapy is an innovative cancer treatment technique that delivers high radiation doses in an extremely short time (≥ 40 Gy/s), inducing the so-called FLASH effect—characterized by the sparing of healthy tissue while maintaining effective tumor control. However, the mechanisms underlying the FLASH effect remain unclear, and ongoing research aims to elucidate them. One approach to investigating this phenomenon is through Monte Carlo simulations of particle transport and the resulting radiolysis in aqueous media, enabling comparisons between FLASH and conventional irradiation.

Methods

To provide a useful tool for investigating the effects of FLASH irradiation, the Geant4-DNA example "UHDR" was introduced in the beta release 11.2.0 of Geant4 (June 2023). This example incorporates a newly developed radiolysis chemical stage based on the diffusion-reaction master equation (RDME), a mesoscopic method that bridges microscopic particle-level interactions and macroscopic chemical kinetics. This approach allows the extension of the simulation time to minutes post-irradiation, enabling the validation of equilibrium processes that may play a crucial role on long time scales. In this context, the impact of pH on radiolytic species yields towards equilibrium is particularly important. For the first time in Geant4-DNA, the UHDR example allows taking into account the effect of different pH values on water radiolysis.

Results

This study aims to benchmark the capability of the UHDR example to accurately reproduce the effect of pH on radiolytic species yields. Preliminary results are currently under analysis for 1 MeV electron and 300 MeV proton irradiation in the conventional modality, with comparisons against literature data.

Conclusions

The ability to simulate the impact of pH on water radiolysis represents a significant advancement in studying the evolution of radiolytic species toward equilibrium. This improvement could provide valuable insights into potential differences in chemical evolution under FLASH irradiation compared to conventional irradiation.

Fri, Aug 1 09:00–10:30

Multilevel simulation of ensemble Kalman methods: interactions across levels*Toon Ingelaere*

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To solve problems in domains such as filtering, optimization, and posterior sampling, ensemble Kalman methods have recently received much attention. These parallelizable and often gradient-free algorithms use an ensemble of particles that evolve in time, based on a combination of well-chosen dynamics and interaction between the particles. For computationally expensive dynamics, the cost of attaining a high accuracy quickly becomes prohibitive. To improve the asymptotic cost-to-error relation, different multilevel Monte Carlo techniques have been proposed. These methods simulate multiple differently sized ensembles at different resolutions, corresponding different accuracies and costs. While particles within one of these ensembles do interact with each other, a key question is whether and how particles should interact across ensembles and levels. In this talk, we will outline and compare the most common approaches to such multilevel ensemble interactions.

Fri, Aug 1 09:00–10:30

Adaptive Max-EWMA Control Chart with SVR: Monte Carlo Simulation for Run Length Analysis*Muhammad Noor ul Amin*

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In industrial quality control, monitoring process variations is crucial for ensuring product reliability, particularly when dealing with non-normal data distributions. This study proposes an adaptive Max-EWMA control chart integrated with Support Vector Regression (SVR) for the simultaneous monitoring of process mean and variance. The approach utilizes a dynamic smoothing constant predicted by SVR to enhance sensitivity to real-time process shifts. To address non-normality, Weibull-distributed data is transformed into a standard normal form before analysis. The performance of the proposed method is extensively evaluated through Monte Carlo simulations to assess the run length profile under different process shift scenarios. Results demonstrate the effectiveness of the approach in detecting small to moderate shifts, with the linear kernel exhibiting superior balance between sensitivity and stability, making it an optimal choice for industrial applications. The findings highlight the robustness of the proposed control chart and its adaptability in real-time process monitoring.

Mon, Jul 28 15:30–17:30

Halton Sequences, Scrambling and the Inverse Star-Discrepancy*Christian Weiß*

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Halton sequences are classical examples of multi-dimensional low-discrepancy sequences. Braaten and Weller discovered that scrambling strongly reduces their empirical star-discrepancy. A similar approach may be applied to certain multi-parameter subsequences of Halton sequences. Indeed, results from p-adic analysis guarantee that these subsequences still have the theoretical low-discrepancy property while scrambling has strong effects on the empirical star-discrepancy. By optimizing the parameters of these subsequences known empiric bounds for the inverse star-discrepancy can be improved.

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Mon, Jul 28 15:30–17:30

Star discrepancy and uniform approximation under weighted simple and stratified random sampling*Xiaoda Xu*

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We mainly consider two problems in this talk. First, We consider random discrepancy under weighted importance sampling of a class of stratified input. We give the expected L_p -discrepancy ($2 \leq p < \infty$) upper bound in weighted form under a class of stratified sampling. This result contributes to the error estimate of the upper bound of the integral approximation under weighted importance sampling, and our sampling pattern is a stratified input. Second, we discuss the probabilistic star discrepancy for a random double infinite matrix and propose an improvement to the coefficient of an existing result, we mainly use the optimal refined δ -bracketing number so far.

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Carlo importance sampling. *Statist. Probab. Lett.*, 100-106.

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Mon, Jul 28 15:30–17:30

Transport Quasi-Monte Carlo

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Quasi-Monte Carlo (QMC) is a powerful method for evaluating high-dimensional integrals. However, its use is typically limited to distributions where direct sampling is straightforward, such as the uniform distribution on the unit hypercube or the Gaussian distribution. For general target distributions with potentially unnormalized densities, leveraging the low-discrepancy property of QMC to improve accuracy remains challenging. We propose training a transport map to push forward the uniform distribution on the unit hypercube to approximate the target distribution. Inspired by normalizing flows, the transport map is constructed as a composition of simple, invertible transformations. To ensure that RQMC achieves its superior error rate, the transport map must satisfy specific regularity conditions. We introduce a flexible parametrization for the transport map that not only meets these conditions but is also expressive enough to model complex distributions. Our theoretical analysis establishes that the proposed transport QMC estimator achieves faster convergence rates than standard Monte Carlo, under mild and easily verifiable growth conditions on the integrand. Numerical experiments confirm the theoretical results, demonstrating the effectiveness of the proposed method in Bayesian inference tasks.

Mon, Jul 28 15:30–17:30

Using Normalizing Flows for Efficient Quasi-Random Sampling for Copulas

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In finance and risk management, copulas are used to model the dependence between stock

prices and insurance losses to compute expectations of interest. Generally, Monte Carlo (MC) sampling is used to generate copula samples to approximate expectations. To reduce the variance of the approximation, we can use quasi-Monte Carlo (QMC) sampling to generate copula samples. This paper examines a new method to generate quasi-random samples from copulas requiring fewer training resources than previous methods such as the generative moment matching networks (GMMN) model [1]. Traditional methods that do not use generative models often rely on conditional distribution methods (CDM) to generate quasi-random samples from specific copulas [2]. CDM is limited to only a few parametric copulas (Gumbel has no efficient CDM to sample quasi-random samples) in low dimensions [2]. Here, we propose using a powerful and simple generative model called Normalizing Flows (NFs) to generate quasi-random samples for any copula, including cases where we only have data available. NFs are a type of explicit generative model that relies on transforming a simple density, such as a normal density, through efficient invertible transformations that rely on the change of variables formula into a density that models complex data that facilitates easy sampling and efficient inverting of samples from complex data to normal data and vice versa. The benefit of these NFs for copula modelling is that their training is efficient in terms of runtime, allowing for larger batch sizes compared to the GMMN model [1]. Also, it is sample-efficient; it only needs samples from the copula and not samples from the normal as the GMMN model [1] required. Once the NF model is trained, we can efficiently invert the model to take as input quasi-random samples to generate quasi-random copula samples. Through many different simulations and applications, we show our approach allows us to leverage the benefit of QMC in a variety of real-world settings involving dependent data.

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Tue, Jul 29 15:30-17:30

Approximation using median lattice algorithms

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We consider L_2 -approximation of functions in a weighted Korobov space. We present a median algorithm, which is related to median integration rules, that have recently gained a lot of interest in the theory of quasi-Monte Carlo methods. Indeed, we use lattice rules as the underlying integration rules to approximate Fourier coefficients. As we will show, we can obtain a convergence rate that is arbitrarily close to optimal in terms of the number of evaluations needed of the function to be approximated.

Tue, Jul 29 15:30-17:30

Convergence Rates of Randomized Quasi-Monte Carlo Methods under Various Regularity Conditions

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In this work, we analyze the convergence rate of randomized quasi-Monte Carlo (RQMC) methods under Owen's boundary growth condition (Owen, 2006) via spectral analysis. We examine the RQMC estimator variance for two commonly studied sequences—the lattice rule and the Sobol' sequence—using the Fourier transform and Walsh–Fourier transform, respectively. Under certain regularity conditions, our results reveal that the asymptotic convergence rate of the RQMC estimator's variance closely aligns with the exponent specified in Owen's boundary growth condition for both sequence types. We also provide an analysis for certain discontinuous integrands.

In addition, we investigate the L^p integrability of weak mixed first-order derivatives of the integrand and study the convergence rates of scrambled digital nets. We demonstrate that the generalized Vitali variation with parameter $\alpha \in [\frac{1}{2}, 1]$ from Dick and Pillichshammer (2010) is bounded above by the L^p norm of the weak mixed first-order derivative, where $p = \frac{2}{3-2\alpha}$. Consequently, when the weak mixed first-order derivative belongs to L^p for $1 \leq p \leq 2$, the variance of the scrambled digital nets estimator converges at a rate of $\mathcal{O}\left(N^{-4+\frac{2}{p}} \log^{s-1} N\right)$. Together, these results provide a comprehensive theoretical framework for understanding the convergence behavior of RQMC methods and scrambled digital nets under various regularity assumptions.

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Tue, Jul 29 15:30-17:30

Use of rank-1 lattices in the Fourier neural operator*Jakob Dilen*

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The “Fourier neural operator” [2] is a variant of the “neural operator”. Its defining characteristic, compared to the regular neural operator, is that it transforms the input to the Fourier domain at the start of each layer. This transformation uses the d -dimensional FFT on a regular grid in d dimensions. We describe how to do this more efficiently using rank-1 lattice points, which allow for a one-dimensional FFT algorithm, see, e.g., [1].

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- [2] Z. Li, N. B. Kovachki, K. Azizzadenesheli, B. Liu, K. Bhattacharya, A. Stuart, and A. Anandkumar. *Fourier neural operator for parametric partial differential equations*. International Conference on Learning Representations, 2021.

Tue, Jul 29 15:30-17:30

Investigating the Optimum RQMC Batch Size for Betting and Empirical Bernstein Confidence Intervals*Aadit Jain*

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The Betting [1] and Empirical Bernstein (EB) [1,2] confidence intervals (CIs) are finite sample (non-asymptotic) and require IID samples. Since both are non-asymptotic, they are much wider than confidence intervals based on the Central Limit Theorem (CLT) due to the stronger coverage property they provide. To apply these finite sample CIs to randomized quasi-Monte Carlo (RQMC), we take R independent replications of n RQMC points, averaging the n function evaluations within each replication. Given a fixed budget $N = nR$, we investigate the optimal n that minimizes the CI widths for both methods.

Using the code from [1], we ran simulations on various integrands (smooth, rough, one-dimensional, multi-dimensional) and ridge functions. Interestingly, the optimal n was quite small compared to N , often just 1 (plain IID), 2, or 4 when $N = 2^{10}$. Moreover, the optimal n appeared to grow quite slowly as N increased. Notably, both CI methods applied to RQMC

outperformed plain IID when the optimal n is greater than 1.

This experimental trend aligns with our analysis of Bennett’s inequality for EB [2], which suggests that the optimum n is $O(N^{1/(2\theta+1)})$ for $\theta > 1/2$. Specifically, for $\theta = 3/2$, which occurs for smoother integrands, we obtain $n = O(N^{1/4})$. For $\theta = 1$, which corresponds to a typical Koksma-Hlawka rate, we get $n = O(N^{1/3})$. The ratio of RQMC EB CI widths to plain IID EB CI widths is $\Theta(N^{(1-2\theta)/(4\theta+2)})$. For $\theta = 1$, we get a ratio of $\Theta(N^{-1/6})$, while for $\theta = 3/2$, we get a more favorable width ratio of $\Theta(N^{-1/4})$.

On the other hand, CLT based CIs using RQMC are only asymptotically valid. The value of R could be any reasonable number that isn’t too small, and remains constant as the total sample size, N , increases. This means that $n = \Theta(N)$, which takes full advantage of the power of QMC. It is also important to note that both Betting and EB require the random variables to be bounded between 0 and 1, unlike CLT based CIs.

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Wed, Jul 30 10:30-12:30

Sampling with constraints

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We will present first order and second order numerical integrators for reflected (overdamped) Langevin dynamics [1] and confined (underdamped) Langevin dynamics [2], respectively. We show how these SDEs can be used for sampling from a desired measure with compact support. We will also discuss sampling on hyper-surfaces. We will showcase numerical examples to verify the presented results.

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Wed, Jul 30 10:30-12:30

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Hamiltonian Monte Carlo (HMC) is widely used for sampling from high-dimensional target distributions with probability density known up to proportionality. While HMC possesses favorable dimension scaling properties, it encounters challenges when applied to strongly multimodal distributions. Traditional tempering methods, commonly used to address multimodality, can be difficult to tune, particularly in high dimensions. In this study, we propose a method that combines a tempering strategy with Hamiltonian Monte Carlo, enabling efficient sampling from high-dimensional, strongly multimodal distributions. Our approach involves proposing candidate states for the constructed Markov chain by simulating Hamiltonian dynamics with time-varying mass, thereby searching for isolated modes at unknown locations. Moreover, we develop an automatic tuning strategy for our method, resulting in an automatically-tuned, tempered Hamiltonian Monte Carlo (ATHMC). Unlike simulated tempering or parallel tempering methods, ATHMC provides a distinctive advantage in scenarios where the target distribution changes at each iteration, such as in the Gibbs sampler. We numerically show that our method scales better with increasing dimensions than an adaptive parallel tempering method and demonstrate its efficacy for a variety of target distributions, including mixtures of log-polynomial densities and Bayesian posterior distributions for a sensor network self-localization problem.

Wed, Jul 30 10:30-12:30

Localized consensus-based sampling for non-Gaussian distributions*Arne Bouillon*

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Drawing samples distributed according to a given unnormalized probability density function is a common task in Bayesian inverse problems. Algorithms based on an ensemble of interacting *particles*, moving in parameter space, are gaining in popularity for these problems since they are often parallelizable, derivative-free, and affine-invariant. However, most are only accurate for near-Gaussian target distributions; an example is the consensus-based sampling (CBS) method [1]. We propose a novel way to derive CBS from ensemble-preconditioned Langevin diffusions by first approximating the target potential by its anisotropic Moreau envelope, then approximating the proximal operator by a weighted mean, and finally assuming that the initial and target distributions are Gaussian. We adapt these approximations with non-Gaussian distributions in mind and arrive at a new interacting-particle method for sampling, which we call *localized consensus-based sampling*. Numerical tests illustrate that localized CBS compares favorably to alternative methods in terms of affine-invariance and performance on non-Gaussian distributions.

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Wed, Jul 30 10:30-12:30

Importance Sampling for Hawkes Processes*Alex Shkolnik*

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In 1971, Alan Hawkes [1] introduced a highly influential point process N for which, given a constant $\mu > 0$ and a $[0, \infty)$ -valued function g , the intensity process X takes the form,

$$X_t = \mu + \int_0^t g(t-s) dN_s, \quad (t \geq 0). \quad (5.2)$$

By now, Hawkes processes have found a wide array of application in the sciences, engineering, statistics, operations research, mathematical finance and machine learning. We develop importance sampling estimators for rare-event probabilities of the form $\mathbb{P}(N_t \geq ct)$ and

general functions g in (5.2). This problem has received little attention to date, as for most g , the process (N, X) is non-Markovian and lends to little mathematical tractability. Our approach is based on a Girsanov change of intensity coupled with a conditioning on the rare-event. We prove asymptotic optimality of the resulting importance sampling estimators in the limit $t \rightarrow \infty$. Related large deviations results and an extension to fully nonlinear models of N with intensity $\phi(X)$ are presented. Numerical simulations illustrate the performance of our importance sampling estimators relative to Monte Carlo for various functions g as well as to exponential tilting in the case of an exponential g (the sole tractable model).

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Thu, Jul 31 15:30–17:30

Revisiting the Gibbs Sampler: A Conditional Modeling Perspective

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The Gibbs sampler (GS) is a fundamental algorithm for approximating analytically intractable distributions. Two major generalizations of GS are the partially collapsed Gibbs sampler (PCGS) and the pseudo-Gibbs sampler (PGS). For PCGS, the associated Markov chain is heterogeneous with varying state spaces, making traditional convergence analysis challenging. To address this, we introduce the iterative conditional replacement (ICR) algorithm and prove its convergence. Furthermore, ICR provides a systematic approach for approximating multiple stationary distributions arising in PGS. Our approach emphasizes the advantage of treating each conditional density with its own operator, rather than aggregating all conditionals into a single operator.

Thu, Jul 31 15:30–17:30

Concatenation of Markov processes for Monte Carlo Integration

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Markov Chain Monte Carlo (MCMC) is a sophisticated sampling technique used to sample from a probability distribution when conventional methods are impractical. Widely applied in statistics, machine learning, physics, and finance, MCMC generates samples from a probability distribution through an invariant Markov process. However, controlling and fine-tuning the process pose challenges, particularly in achieving both rapid local exploration and global distribution discovery. The Metropolis-Hastings algorithm, the most popular MCMC technique, while practical, struggles to excel in these objectives due to its inherent reversibility, leading to diffusive exploration and the need for large-scale perturbations for global discovery.

Wang et al. [2] introduced a novel MCMC approach, which is based on the concatenation of Markov processes [1]. It allows the usage of an essentially arbitrary Markov process for local exploration. That way, the process can be chosen to satisfy a desired exploration behavior suitable for the state space at hand without worrying about invariance at this point. The process is executed up to a certain finite lifetime. After this time has elapsed, the process is *killed* and started afresh at a spawn location drawn from a *regeneration* distribution. The lifetime is chosen in a way ensuring that the overall process is invariant with respect to a given target distribution.

We generalize this idea and introduce it with appropriate rigor. We show how the validity of the method can be established for a more general class of Markov processes. We also allow the usage of a whole family of Markov processes for local exploration with possibly varying exploration characteristic. We establish a transfer mechanism between consecutive processes, which allows the user to specify the initial state of the newly spawned process to depend on the exit point of the previous one. Not least, we derive a Rao-Blackwellization technique which guarantees variance reduction in practice. We showcase the potential of the framework in a practical rendering experiment. We compare the method proposed in [2] with existing methods based on Metropolis-Hastings algorithms with Random-Walk, Langevin and Hamiltonian proposals, respectively.

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Thu, Jul 31 15:30–17:30

Polynomial approximation for efficient transport-based sampling*Josephine Westermann*

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Sampling from non-trivial probability distributions is a fundamental challenge in uncertainty quantification and inverse problems, particularly when dealing with high-dimensional domains, costly-to-evaluate or unnormalized density functions, and non-trivial support structures. Measure transport via polynomial density surrogates [1] provides a systematic and constructive solution to this problem by reformulating it as a convex optimization task with deterministic error bounds. This approach is particularly efficient for smooth problems but can become computationally demanding when dealing with highly concentrated posterior distributions, as constructing the density surrogate requires many evaluations in regions where the density is nearly zero—leading to an inefficient allocation of computational resources. In this talk, we explore how the computational cost in such cases can be further reduced by first approximating the potential function with a polynomial. This additional approximation step shifts the focus of expensive evaluations toward capturing the underlying system more effectively. The surrogate-based posterior can then be evaluated cheaply and approximated with high accuracy, enabling efficient transport-based sampling. We discuss the implications of this strategy and examine its potential to enhance performance in demanding inference problems.

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Thu, Jul 31 15:30–17:30

Fast Approximate Matrix Inversion via MCMC for Linear System Solvers*Soumyadip Ghosh*

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A key prerequisite of modern iterative solvers of linear algebraic equations $Ax = b$ is the fast computation of a pre-conditioner matrix P that gives a good approximation to the (generalized) inverse of A such that the set of equations obtained by pre-multiplying with P , $PAx = Pb$, is solved quickly. We study the classical Ulan-von Neumann MCMC algorithm that was designed based on the Neumann infinite series representation of the inverse of a non-singular matrix. The parameters of the MCMC algorithm determine the overall time to solve

$Ax = b$, which is a metric that reflects both the time to compute the MCMC preconditioner P and its quality as a preconditioner to solve the linear equations. Our main focus is on how the MCMC parameters should be tuned to speed up computations in applications that require repeated calls to the solver with varying matrices A , a common scenario for instance in numerical approximations of physical phenomena. We present a model that relates key features of matrices A with good choices of MCMC algorithm parameters that lead to a fast overall time to find a solution to $Ax = b$. A computationally efficient approach based on Bayesian experimental design is described to learn and update this model while minimizing the number of runs of the expensive solver in application settings that solve of linear system over well defined sets of A matrices. We present numerical experiments to illustrate the efficacy of this approach. In another contribution, we present a new MCMC algorithm which we term as *regenerative Ulam-von Neumann* algorithm. It exploits a regenerative structure present in the Neumann series that underlies the original algorithm and improves on it by producing an unbiased estimator of the matrix inverse. A rigorous analysis of performance of the algorithm is provided. This includes the variance of the estimator, which allows one to estimate the time taken to obtain solutions of a desired quality. Finally, numerical experiments verify the qualitative effectiveness of the proposed scheme.

Thu, Jul 31 10:30–12:30

The Stochastic Differential Equations of the Heston Model for Option Pricing

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The Heston model is a widely used stochastic volatility model for option pricing, addressing the limitations of the Black-Scholes model by incorporating a stochastic variance process. This talk will cover the stochastic differential equations (SDEs) governing the Heston model, demonstrating their application in option pricing.

The Heston model introduces a stochastic process for volatility, improving the accuracy of derivative pricing. The dynamics of the asset price S_t and its variance v_t under the Heston model are given by[1]:

$$dS_t = \mu S_t dt + \sqrt{v_t} S_t dW_t^S, \quad (5.3)$$

$$dv_t = \kappa(\theta - v_t)dt + \sigma\sqrt{v_t}dW_t^v, \quad (5.4)$$

where:

- μ is the drift of the asset price.
- κ is the rate of mean reversion of variance v_t towards long-term mean θ .
- σ represents the volatility of volatility.

- dW_t^S and dW_t^v are Wiener processes with correlation ρ .

We will explore Monte Carlo methods as a numerical approach to simulate price paths and compute option prices for European and American derivatives [2],[3]. Furthermore, an interactive Shiny web application will be presented, showcasing real-time simulations and visualizations of option pricing under the Heston framework.

An interactive web-based application is implemented using Shiny in R, enabling users to:

- Adjust input parameters $(S_0, K, r, T, \mu, \theta, \kappa, \sigma, \rho)$.
- Perform Monte Carlo simulations to compute option prices.
- Visualize option price distributions and convergence results.

The Shiny application offers an interactive tool for financial analysis. Future work may explore enhancements such as incorporating jump-diffusion models and GPU-accelerated simulations.

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Thu, Jul 31 10:30–12:30

Characterizing Efficacy of Geometric Brownian Motion Expectation-based Simulations on Low-Volatility American Common Stocks

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In this manuscript, daily, monthly, and annual geometric Brownian motion forecasts are obtained and tested for reliability upon 21 stock symbols within NASDAQ of varying volatilities and drifts. Biweekly, monthly, biannual, and annual rolling windows were used as a preliminary filtering scheme to remove unreliable stock symbols, and then accuracy was further evaluated on stocks with higher accuracies in the first screening. Annual and 10-year windows were used to estimate the drift and diffusion component and then applied to obtain one-period-ahead geometric Brownian motion stock values and associated probabilities. Further building off of these one-period-ahead values, expected values for 1-252 periods were estimated. Expected values of each stock were estimated by totaling up the product of the stock value and its associated probabilities, and tested over multiple rolling-windows for

reliability. The results indicate that geometric Brownian-simulated expected index values estimated using one thousand simulations can be slightly reliable if catered and re-optimized to specific stock characterizations, but only for a daily window, and even then only slightly preferable to flipping a coin. Expected values estimated with less than 100 simulations were thrown out, seen as unreliable.

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Thu, Jul 31 10:30–12:30

Efficient Pricing for Variable Annuity via Simulation*Hao Quan*

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Variable Annuities (VAs) are insurance products that offer policyholders exposure to financial market upside potential while safeguarding against downside risk through optional riders, such as Guaranteed Minimum Death Benefits (GMDBs), Guaranteed Minimum Accumulation Benefits (GMABs), and Guaranteed Minimum Withdrawal Benefits (GMWBs). These riders, tailored to policyholders' needs, introduce a complex risk profile combining mortality and financial uncertainties, rendering VA pricing and fee determination computationally challenging. Due to this complexity, Monte Carlo simulation is often the only practical approach for valuing these contracts.

In this study, we address the problem of setting fair management fees for VA rider combinations using the equivalence principle, which balances the expected present value of premiums and benefits. We formulate fee determination as a stochastic root-finding problem, expressed as

$$E[V(\varphi)] - P = 0,$$

where $E[V(\varphi)]$ denotes the expected present value of VA benefits under fee structure φ , and P represents the premium. The VA benefit $V(\varphi)$ reflects the evolution of the contract's shadow account value and various benefit guarantees over the contract's lifetime. As a result, estimating its expected value is computationally challenging. Moreover, solving the root-finding problem requires estimating the gradient of this expectation. To solve this, we employ stochastic gradient estimation techniques, such as finite differences and infinitesimal perturbation analysis (IPA). We analyze the theoretical properties and computational performance of the proposed root-finding algorithms, offering insights into their efficacy for VA pricing. Our results show that gradient estimation techniques have a significant impact on the efficiency and accuracy of estimating fair fees for various rider combinations.

Fri, Aug 1 09:00–10:30

Revisiting self-normalized importance sampling: new methods and diagnostics*Nicola Branchini*

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Importance sampling (IS) can often be implemented only with normalized weights, yielding the popular self-normalized IS (SNIS) estimator. However, proposal distributions are often

learned and evaluated using criteria designed for the unnormalized IS (UIS) estimator.

In this talk, we aim to present a unified perspective on recent methodological advances in understanding and improving SNIS. We propose and compare two new frameworks for adaptive importance sampling (AIS) methods tailored to SNIS. Our first framework exploits the view of SNIS as a ratio of two UIS estimators, coupling two separate AIS samplers in a joint distribution selected to minimize asymptotic variance. Our second framework instead proposes the first MCMC-driven AIS sampler directly targeting the (often overlooked) optimal SNIS proposal.

We also establish a close connection between the optimal SNIS proposal and so-called subtractive mixture models (SMMs), where negative coefficients are possible - motivating the study of the properties of the first IS estimators using SMMs.

Finally, we propose new Monte Carlo diagnostics specifically for SNIS. They extend existing diagnostics for numerator and denominator by incorporating their statistical dependence, drawing on different notions of tail dependence from multivariate extreme value theory.

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Fri, Aug 1 09:00–10:30

Quantitative results on sampling from quasi-stationary distributions

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We study the rate of convergence of Sequential Monte Carlo (SMC) methods for approximating the quasi-stationary distribution (QSD) of Markov processes. For processes with killing or absorption, the QSD appears as a stable behavior observed before extinction, or as the limiting distribution of the process conditioned on not being absorbed. We give quantitative lower and upper bounds for the particle filter approximation of these distributions. For the lower bound, we show that fast mixing is not enough to guarantee that simulation methods

can converge in few steps. In the upper bound, we show that SMC with adaptive resampling has a rate depending on the number of steps, the mixing time, and in how fast the processed gets killed. Our seems to be the first result to have a quantitative dependency of this form that is valid for discrete time Markov chains in general state spaces. Our techniques and concentration results for bounding the approximations of SMC with adaptive resampling are also novel, and we believe might be applicable in other scenarios that can benefit from the lower variance obtained due to an adaptive approach.

Fri, Aug 1 09:00–10:30

Serial ensemble filtering with marginal coupling

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Serial filtering refers to a univariate, state by state Bayesian inference problem. Extant methods for serial filtering result in suboptimal posterior samples for severely non-Gaussian, multimodal inference settings. We fix this problem by rigorously coupling the state marginal densities with information about their joint density. This formulation allows for accurately sampling the Bayesian posterior across a variety of challenging text problems.

Wed, Jul 30 14:00–16:00

Stochastic gradient Langevin dynamics with non-stationary data

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We investigate the mixing properties of the stochastic gradient Langevin dynamics (SGLD) algorithm with a fixed step size. While most existing studies on SGLD assume an i.i.d. data stream, this assumption is often unrealistic in practical applications, such as financial time series analysis, natural language processing, and sensor data processing. In such settings, the sequence of iterates no longer forms a Markov chain, significantly complicating the

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mathematical analysis [1, 2].

To address this challenge, we model the iterates as a Markov chain in a random environment (see [4, 5], and [6]). Under standard dissipativity and Lipschitz conditions, we establish the transfer of α -mixing properties from the data stream to the sequence of iterates [3]. This enables us to derive key theoretical results, including the law of large numbers, the central limit theorem, and concentration inequalities for SGLD in the non-convex setting. Our findings provide theoretical guarantees for SGLD in a more realistic scenario where the data merely weakly dependent.

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Wed, Jul 30 14:00–16:00

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Tim Johnston, Nikos Makras, Sotirios Sabanis

In this article, we study the problem of sampling from distributions whose densities are not necessarily smooth nor log-concave. We propose a simple Langevin-based algorithm that does not rely on popular but computationally challenging techniques, such as the Moreau Yosida envelope or Gaussian smoothing. We derive non-asymptotic guarantees for the convergence of the algorithm to the target distribution in Wasserstein distances. Non asymptotic bounds are also provided for the performance of the algorithm as an optimizer, specifically for the solution of associated excess risk optimization problems.

Possible extensions to potentials with log-gradients that grow super-linearly may also be discussed.

This is based on the joint work in [1].

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Wed, Jul 30 14:00–16:00

Langevin-based strategies for nested particle filters

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Many problems in some of the most active fields of science require to estimate parameters and predict the evolution of complex dynamical systems using sequentially collected data. The nested particle filter (NPF) framework stands out since it is the only fully recursive probabilistic method for Bayesian inference. That is, it computes the joint posterior distribution of the parameters and states while maintaining a computational complexity of $\mathcal{O}(T)$, which makes it particularly suitable for long observation sequences.

A key strategy to keep particle diversity in the parameter space, given the static nature of the parameters, is jittering. The parameter space is explored by perturbing a subset of particles with arbitrary variance or applying a controlled variance to all particles. As the perturbations are controlled, it ensures convergence to the true posterior distribution while keeping the full framework recursive. However, this is not an efficient exploration strategy, particularly for problems with a higher dimension in the parameter space.

To address this limitation, we propose a Langevin-based methodology within the NPF framework. A challenge is that the required score function is intractable. We propose to approximate the score with an accurate method that is provably stable over time, and to explore strategies to reduce its computational cost while retaining accuracy. This approach significantly improves the scalability of NPF in the parameter dimension, while still ensuring asymptotic convergence to the true posterior, as well as maintaining computational feasibility.

Wed, Jul 30 14:00–16:00

Taming the Interacting Particle Langevin Algorithm – The Superlinear Case*Nikolaos Makras*

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Recent advances in stochastic optimization have yielded the interacting particle Langevin algorithm (IPLA), which leverages the notion of interacting particle systems (IPS) to efficiently sample from approximate posterior densities. This becomes particularly crucial in relation to the framework of Expectation-Maximization (EM), where the E-step is computationally challenging or even intractable. Although prior research has focused on scenarios involving convex cases with gradients of log densities that grow at most linearly, our work extends this framework to include polynomial growth. Taming techniques are employed to produce an explicit discretization scheme that yields a new class of stable, under such non-linearities, algorithms which are called tamed interacting particle Langevin algorithms (tIPLA). We obtain non-asymptotic convergence error estimates in Wasserstein-2 distance for the new class under the best known rate.

- [1] Tim Johnston, Nikolaos Makras and Sotirios Sabanis, *Taming the Interacting Particle Langevin Algorithm – The Superlinear Case* (2024). Preprint: arxiv:2403.19587

Thu, Jul 31 15:30-17:30

Dynamical Low-Rank Approximation for SDEs: an interacting particle-system ROM*Fabio Zoccolan*

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The Dynamical Low-Rank Approximation (DLRA) technique is a time-dependent reduced-order model (ROM) known for its significant advantages in terms of computational time and accuracy. Its appeal in uncertainty quantification is due to the fact that its solution is composed of time-dependent deterministic and stochastic bases, allowing the approximation to better track the dynamics of the studied system. In the context of stochastic differential equations (SDEs) a rigorous mathematical setting was presented in [1], using the so-called Dynamically Orthogonal (DO) framework. The well-posedness of this setting is nontrivial due to the coupled nature of the DO system: for instance, the deterministic basis depends on all stochastic basis paths, and the equations involve the inversion of a Gramian matrix.

When coming to stochastic discretization through a Monte-Carlo procedure, these features imply to deal with a interacting noisy particle dynamics. We proposed two fully discretized schemes based on the Monte-Carlo method, investigating their errors and analyzing possible issues arisen by the discretization of the Gramian inverse [2]. Theoretical results will be supported by numerical simulations.

- [1] Yoshihito Kazashi, Fabio Nobile, and Fabio Zoccolan. *Dynamical low-rank approximation for stochastic differential equations*. Mathematics of Computation (2024).
- [2] Yoshihito Kazashi, Fabio Nobile, and Fabio Zoccolan. *Numerical Methods for Dynamical low-rank approximation of stochastic differential equations, Part I & II*, in preparation (2025).

Thu, Jul 31 15:30-17:30

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Stochastic differential equations driven by Lévy processes have become established as models to describe the evolution of random variables such as financial and economic variables and more recently of climate variables, when the stochastic system shows jump discontinuities. In this talk, we derive a novel series representation of the flowmap of such stochastic differential equations in terms of commutators of vector fields with stochastic coefficients, in other words a Chen–Strichartz formula. We provide an explicit expression for the components in this series. Our results extend previous results for deterministic and continuous stochastic differential equations.

Thu, Jul 31 15:30-17:30

Comparing Probabilistic Load Forecasters: Stochastic Differential Equations and Deep Learning

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Generating probabilistic predictions for the electricity-load profile is the foundation of efficient use of renewable energy and diminishing carbon footprint.

In this talk, we consider the problem of creating probabilistic forecasts of the day-ahead electricity consumption profile of an agglomerate of buildings in the city of Lausanne (Switzerland) in the absence of an externally provided prediction function.

We propose a nonparametric, data-driven, approach based on Itô' Stochastic Differential Equations (SDEs) [1]. Our work is novel in that the mean function of the SDE is expanded on a Fourier periodic basis, capturing intra-day and intra-week periodic features. Using a derivative tracking term, we impose the trajectories of the process to revert toward the mean. To model high-volatility levels associated with more uncertain electricity consumption regimes, we employ a square-root type diffusion coefficients.

Maximum-Likelihood estimation is used to infer the parameters of the model coherently with the available observations of the time history. We show that the maximization problem is well posed and that it admits at least one solution over the feasible domain.

We compare the probabilistic predictions generated by the SDE with Deep Learning based probabilistic forecaster. On the one hand, we introduce a Deep Learning forecaster based on Long short-term memory (LSTM) recurrent neural networks trained by minimizing the quantile loss function. This approach allows the generation of confidence intervals by sampling from the one-step-ahead univariate cumulative density function (CDF) associated with the electricity consumption of the future time instant. On the other hand, inspired by [2], we consider Multivariate Quantile Function Forecasters that, based on Normalizing Flows, learn the multivariate cumulative density function of the day-ahead electricity consumption.

Metrics such as Continuous ranked probability score and Prediction interval coverage percentage are used to assess the quality of the forecasts.

We show that SDEs generate reliable and interpretable predictions while presenting the most parsimonious and computationally efficient structure among the three models.

- [1] Riccardo Saporiti, Fabio Nobile, Celia García-Pareja. *Probabilistic Forecast of the Day-Ahead electricity consumption profile with Stochastic Differential Equations: a comparison with Deep Learning models*. In preparation.
- [2] Kelvin Kan, Francois-Xavier Aubet, Tim Januschowski, Youngsuk Park, Konstantinos Benidis, Lars Ruthotto, and Jan Gasthaus (2022). *Multivariate Quantile Function Forecaster*. Proceedings of The 25th International Conference on Artificial Intelligence and Statistics, PMLR 151:10603-10621, 2022.

Thu, Jul 31 15:30-17:30

Forward Propagation of Low Discrepancy Through McKean–Vlasov Dynamics: From QMC to MLQMC*Leon Wilkosz*

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This work develops a particle system addressing the approximation of McKean–Vlasov stochastic differential equations (SDEs). The novelty of the approach lies in involving low discrepancy sequences nontrivially in the construction of a particle system with coupled noise and initial conditions. Weak convergence for SDEs with additive noise is proven. A numerical study demonstrates that the novel approach presented here doubles the respective convergence rates for weak and strong approximation of the mean-field limit, compared with the standard particle system. These rates are proven in the simplified setting of a mean-field ordinary differential equation in terms of appropriate bounds involving the star discrepancy for low discrepancy sequences with a group structure, such as Rank-1 lattice points. This construction nontrivially provides an antithetic multilevel quasi-Monte Carlo estimator. An asymptotic error analysis reveals that the proposed approach outperforms methods based on the classic particle system with independent initial conditions and noise.

Mon, Jul 28 15:30-17:30

A probabilistic Numerical method for semi-linear elliptic Partial Differential Equations

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EmmanuelGobet, CharuShardul, LukaszSzpruch

In this presentation, we study the numerical approximation of a class of Backward Stochastic Differential Equations (BSDEs) in an infinite horizon setting that provide a probabilistic representation for semi-linear elliptic Partial Differential Equations. In particular, we are also able to treat some ergodic BSDEs that are related to elliptic PDEs or ergodic type. In order to build our numerical scheme, we put forward a new representation of the PDE solution by using a classical probabilistic representation of the gradient. Then, based on this representation, we propose a fully implementable numerical scheme using a Picard iteration procedure, a grid space discretization and a Monte-Carlo approximation. We obtain an upper bound for the numerical error and we also provide some numerical experiments that show the efficiency of this approach for small dimensions. Some numerical experiments also show that it is possible to efficiently handle larger dimensions by replacing grid-based spatial discretization with neural networks. This presentation is based on [1] for the non ergodic framework and [2] for results concerning the ergodic case.

- [1] Gobet, Emmanuel, & Richou, Adrien, & Shardul, Charu (2025). Numerical approximation of Markovian BSDEs in infinite horizon and elliptic PDEs. Draft.
- [2] Gobet, Emmanuel, & Richou, Adrien, & Szpruch, Lukasz (2025). Numerical approximation of ergodic BSDEs using non linear Feynman-Kac formulas, Preprint arXiv:2407.09034

Mon, Jul 28 15:30-17:30

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As is known, the nonlinear Boltzmann equation describes the behavior of rarefied gas much better than the linear Kac's [1] model. That is why we can expect that application of the nonlinear spatially homogenous Boltzmann equation to the Harlow's "particles-in-cell" model [2] allows us to do a computation, which gives a more exact approximation of the solution. Among the statistical methods [3], which use Monte Carlo directly for modeling the flow of rarefied gas, the most efficient one is the statistical method of direct modeling the nonstationary flow. In the known "particle-in-cell" method, the simulations divide into

two steps. Monte Carlo method is used both for the numerical simulation of collisions of the particles in cells (the first step), as well as for the collision-free moving of particles (the second step). In this work we propose another computational scheme, which directly uses the non-linear spatially homogenous Boltzmann equation for the numerical realization of the first step in the “particles-in-cell” model of Belotserkovski-Yanitskii [3]. Proposed a new approach of constructing unbiased estimators will give relatively small variance. For this aim we construct a branching Markov process [4] and on its trajectory we propose various “conjugated” computational schemes for calculating an unbiased estimator of the given functional. It should be noted nowadays in this area became popular adjoint direct simulation Monte Carlo method to a general collision kernel [5]. The results of our computations show that they are similar with known Belotserkovski-Yanitskii solutions of the Boltzmann equation. We note that in the interval, where the Boltzmann equations “work” (intermediate interval), the “particle-in-cell” statistical model approximates the spatially heterogeneous Boltzmann equation better.

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Mon, Jul 28 15:30-17:30

A New Approach for Unbiased Estimation of Parameters of Partially Observed Diffusions

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In this talk, we consider the estimation of static parameters for a partially observed diffusion process with discrete-time observations over a fixed time interval. We develop particle filtering methods using time-discretization schemes, and we employ particle Markov chain Monte

Carlo methods to estimate the smoothing distribution. In particular, we use backward sampling to address the issue of sample degeneracy. We use the score function and stochastic gradient ascent methods to maximize the likelihood of the observations. Parameter estimation in the diffusion term is possible by introducing bridge processes and the corresponding bridge-guiding proposals. To achieve an unbiasedness, we adopt the Rhee and Glynn approach [1], in which the sources of bias are the number of stochastic gradient ascent steps and the time-discretization. Finally, we display numerically the method applying it to two systems.

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Mon, Jul 28 15:30-17:30

High-order adaptive methods for exit times of diffusion processes and reflected diffusions

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The Feynman–Kac formula connects domain-exit and boundary-reflection properties of stochastic differential equations (SDEs) and parabolic partial differential equations. The SDE viewpoint is particularly interesting for numerical methods, as it can be used with Monte Carlo methods to overcome the curse of dimensionality when solving high-dimensional PDE. This however hinges on having an efficient numerical method for simulating the exit times of SDEs. Since exit times of diffusion processes are very sensitive to perturbations in initial conditions, it is challenging to construct such numerical methods.

This talk presents a high-order method with adaptive time-stepping for strong approximations of exit times. The method employs a high-order Itô–Taylor scheme for simulating SDE paths and carefully decreases the step size in the numerical integration as the diffusion process approaches the domain’s boundary. These techniques complement each other well: adaptive time-stepping improves the accuracy of the exit time by reducing the overshoot out of the domain, and high-order schemes improve the state approximation of the diffusion process, which is useful feedback to control the step size. We will also consider an ongoing extension of the numerical method to reflected diffusions.

Thu, Jul 31 10:30-12:30

Learning cooling strategies in simulated annealing through binary interactions*Frédéric Blondeel*

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Global optimization is amongst the hardest to solve problems. This is because finding the global minimum can usually only be guaranteed to be found in infinite time. Therefore one usually relies on meta-heuristic algorithms to guide the search and improve chances of successfully identifying the minimum. One particular family of algorithms is simulated annealing (SA). This family of algorithms is inspired by real-world metallurgy and is based on the Metropolis-Hastings algorithm. It works by randomly sampling N particles on the search space, each with a given temperature T . The movement of these particles is analogous to a Brownian random walk with step size proportional to temperature. The temperature is gradually cooled down over the course of the simulation according to some predefined schedule. Due to the Metropolis-Hastings-like acceptance-rejection rule, these particles can jump out of local minima and are expected to move towards the lowest energy state, i.e., the global minimum. It is the design of these cooling schedules for SA that we wish to improve. This is because they directly impact the efficiency of the optimization tool. Typically cooling schedules are inverse logarithmic or geometric decays in time. Here, we consider a collective SA dynamic where particles *interact* to learn the optimal temperature cooling strategy. This is inspired by the well-known particle-swapping technique known as parallel tempering (PT). To this aim we introduce a Boltzmann-type description where particles (partially) exchange their temperatures, therefore slowly cooling down the overall mean temperature. In order to simulate the dynamic we use a direct simulation Monte Carlo (DSMC) algorithm known as Nanbu-Babovsky. We show on various test functions (Ackley, Rastrigin, etc.) that this novel approach outperforms the standard SA with logarithmic and geometric annealing schedules.

Thu, Jul 31 10:30-12:30

Accuracy of Discretely Sampled Stochastic Policies in Continuous-Time Reinforcement Learning*Du Ouyang*

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How to execute a stochastic policy in continuous-time environments is crucial for real-time operations and decision making. We show that, by sampling actions from a stochastic policy

at a fixed time grid and then executing a piecewise constant control process, the controlled state process converges to the corresponding aggregated dynamics in the weak sense as the grid size shrinks to zero and obtain the convergence rate. Specifically, under sufficiently regular conditions on the coefficients, the optimal convergence rate of $O(|\mathcal{G}|)$ is achieved with respect to the time grid \mathcal{G} . For less regular coefficients, a convergence rate is established that varies according to the degree of regularity of the coefficients. Additionally, we also derive large deviation bounds for the weak error. Beyond weak error convergence, strong convergence results are proved with a convergence order of $O(|\mathcal{G}|^{1/2})$ in cases where volatility is uncontrolled. Furthermore, we provide a counterexample to demonstrate that no strong convergence occurs when volatility is controlled. Based on these results, we analyze the bias and variance of the policy evaluation and policy gradient estimators in various algorithms for continuous-time reinforcement learning caused by discrete sampling.

Thu, Jul 31 10:30-12:30

Martingale deep neural networks for quasi-linear PDEs and stochastic optimal controls in 10,000 dimensions

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Coauthor(s): Shuixing Fang, Wenzhong Zhang, Tao Zhou

Abstract: In this talk, we will present a highly parallel and derivative-free martingale neural network method, based on the probability theory of Varadhan's martingale formulation of PDEs, to solve Hamilton-Jacobi-Bellman (HJB) equations arising from stochastic optimal control problems (SOCs), as well as general quasilinear parabolic partial differential equations (PDEs). In both cases, the PDEs are reformulated into a martingale problem such that loss functions will not require the computation of the gradient or Hessian matrix of the PDE solution, and can be computed in parallel in both time and spatial domains. Moreover, the martingale conditions for the PDEs are enforced using a Galerkin method realized with adversarial learning techniques, eliminating the need for direct computation of the conditional expectations associated with the martingale property. For SOCs, a derivative-free implementation of the maximum principle for optimal controls is also introduced. The numerical results demonstrate the effectiveness and efficiency of the proposed method, which is capable of solving HJB and quasilinear parabolic PDEs accurately and fast in dimensions as high as 10,000.

- [1] Cai, Wei, Shuixin Fang, Wenzhong Zhang, Tao Zhou, Martingale deep learning for very high dimensional quasi-linear partial differential equations and stochastic optimal controls, arXiv:2408.14395, August, 2024.

Thu, Jul 31 10:30-12:30

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KarstenNaert,DirkNuyens

Minimizing a function with limited sample points is challenging when function evaluations are costly. We propose a fast interpolation-based approach using the Fast Fourier Transform (FFT) to estimate the minimum more efficiently. By interpolating from a sparse set of samples, our method achieves high accuracy with significantly fewer function evaluations. Preliminary results demonstrate its effectiveness for smooth periodic functions.

Fri, Aug 1 09:00–10:30

Delayed Acceptance Slice Sampling: A Two-Level method for Improved Efficiency in High-Dimensional Settings*Kevin Bitterlich*

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Slice sampling is a Markov chain Monte Carlo (MCMC) method for drawing (approximately) random samples from a posterior distribution that is typically only known up to a normalizing constant. The method is based on sampling a new state on a slice, i.e., a level set of the target density function. Slice sampling is especially interesting because it is tuning-free and guarantees a move to a new state, which can result in a lower autocorrelation compared to other MCMC methods. However, finding such a new state can be computationally expensive due to frequent evaluations of the target density, especially in high-dimensional settings. To mitigate these costs, we introduce a delayed acceptance mechanism that incorporates an approximate target density for finding potential new states. We will demonstrate the effectiveness of our method through various numerical experiments and outline an extension of our two-level method into a multilevel framework.

Fri, Aug 1 09:00–10:30

Gradient-based MCMC in high dimensions*Reuben Cohn-Gordon*

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Sampling from distributions over \mathbb{R}^d for d larger than 10^4 arises as a computational challenge in many of the physical sciences, including particle physics [1], condensed matter physics [2], cosmology [3] and chemistry [4], as well as in Bayesian statistics and machine learning [5]. Commonly used gradient-based variants of Markov Chain Monte Carlo such as Hamiltonian Monte Carlo (HMC) [6] and in particular the No U-Turn Sampler [7], are designed for differentiable multivariate densities, but struggle in very high dimensions. We propose a general purpose approach to the gradient-based high dimensional regime, based on two insights. First, in high dimensional cases where limited asymptotic bias is acceptable, Markov Chain algorithms without Metropolis-Hastings (MH) adjustment are more statistically efficient; we provide theoretical and numerical evidence for this claim and show how to choose a step size to limit the incurred bias to an acceptable level. Second, in the case that MH adjustment is required, we show that a particular 4th order integrator [8] drastically improves the statistical efficiency of HMC and related algorithms in high dimensions.

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Fri, Aug 1 09:00–10:30

Parallel Affine Transformation Tuning: Drastically Improving the Effectiveness of Slice Sampling

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The performance of MCMC samplers tends to depend on various properties of the target distribution, such as its covariance structure, the location of its probability mass, and its tail behavior. We propose *parallel affine transformation tuning* (PATT) [1], a methodological framework that relies on bijective affine transformations, a latent space construction, the adaptive MCMC principle, and interacting parallel chains, and acts as an intermediate layer between the target distribution and an MCMC method applied to it. By transforming a challenging target into a simpler one, PATT can harness the full potential of the underlying MCMC method.

According to our numerical experiments, PATT is particularly effective in its combinations with *elliptical slice sampling* (ESS) [2] and *Gibbsian polar slice sampling* (GPSS) [3]. For targets that are sufficiently well-behaved (e.g. posteriors in Bayesian logistic regression), these combinations produce samples of (empirically) dimension-independent quality at remarkably low computational cost, with PATT-ESS performing best for light-tailed targets and PATT-GPSS being the superior choice for heavy-tailed ones.

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Fri, Aug 1 09:00–10:30

Low-Rank Thinning*Annabelle Michael Carrell*

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The goal in thinning is to summarize a dataset using a small set of representative points. Remarkably, sub-Gaussian thinning algorithms like Kernel Halving and Compress can match the quality of uniform subsampling while substantially reducing the number of summary points. However, existing guarantees cover only a restricted range of distributions and kernel-based quality measures and suffer from pessimistic dimension dependence. To address these deficiencies, we introduce a new low-rank analysis of sub-Gaussian thinning that applies to any distribution and any kernel, guaranteeing high-quality compression whenever the kernel or data matrix is approximately low-rank. To demonstrate the broad applicability of the techniques, we design practical sub-Gaussian thinning approaches that improve upon the best known guarantees for approximating attention in transformers, accelerating stochastic gradient training through reordering, and distinguishing distributions in near-linear time.

Wed, Jul 30 10:30–12:30

Combining quasi-Monte Carlo with Stochastic Optimal Control for Trajectory Optimization of Autonomous Vehicles in Mine Counter Measure Simulations*Philippe Blondeel*

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Modelling and simulating mine countermeasures (MCM) search missions performed by autonomous vehicles is a challenging endeavour. The goal of these simulations typically consists of calculating trajectories for autonomous vehicles in a designated zone such that the coverage (residual risk) of the zone is below a certain user defined threshold. We have chosen to model and implement the MCM problem as a stochastic optimal control problem, see [1]. Mathematically, the MCM problem is defined as minimizing the total mission time needed to survey a designated zone Ω for a given residual risk of not detecting sea mines in the user-chosen square domain, i.e.,

$$\min T_f, \tag{5.5}$$

subjected to

$$\mathbb{E}[q(T_F)] := \int_{\Omega} e^{-\int_0^{T_F} \gamma(\mathbf{x}(\tau), \boldsymbol{\omega}) d\tau} \phi(\boldsymbol{\omega}) d\boldsymbol{\omega} \leq \text{Residual Risk}. \tag{5.6}$$

The output of our stochastic optimal control implementation consists of an optimal trajectory in the square domain for the autonomous vehicle. As shown in Eq. (5.6), the residual risk is mathematically represented as an expected value integral. In [2], we presented a novel relaxation strategy for the computation of the residual MCM risk, used in our stochastic optimal control formulation. This novel relaxation strategy ensures that the residual risk obtained at the end of the optimisation run is below the maximally allowed user requested residual risk. This was however not the case with our initial ‘naive’ implementation of the MCM problem. Our proposed relaxation strategy ensures that the user requested risk is satisfied by sequentially solving the stochastic optimal control problem with an ever increasing size of the domain. We combine this strategy with a quasi-Monte Carlo sampling scheme based on a Rank-1 Lattice rule for the computation of the expected value integral. We observe a speedup up to a factor two in terms of total computational cost in favour of quasi-Monte Carlo when compared to standard Monte Carlo.

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Wed, Jul 30 10:30–12:30

A Monte Carlo Approach to Designing a Novel Sample Holder for Enhanced UV-Vis Spectroscopy

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UV-Vis spectroscopy is one of the most widely used techniques for identifying and quantifying substances in water and other solvents due to its speed and reliability. Its applications span diverse scientific fields, including chemistry, biochemistry, and medicine, as well as industrial sectors such as the pharmaceutical and food industries. Moreover, it plays a crucial role in environmental monitoring, particularly in assessing water quality. While alternative methods such as Raman and Ring Down spectroscopy have emerged, the core design of UV-Vis spectrometers has remained largely unchanged since their inception. Typically, these instruments employ a light source, a monochromator, a standard 1 cm cuvette as the sample holder, and one or more photosensors.

In this work, we present a novel approach that leverages Monte Carlo simulation to optimize the design of the sample holder for enhanced UV-Vis spectroscopy. In particular, our

setup adopts a pulsed light source and a Silicon Photomultiplier (SiPM) with single-photon counting capability. Using the optical transport package available in the Geant4 toolkit, we characterized and optimized the new design. The innovative holder, crafted in PTFE for its high UV reflectivity, resembles an integrating sphere, which increases the photon path length in the solution and thereby enhances absorbance in the presence of absorbing substances. We also present a comparison between experimental data and Monte Carlo predictions for validation. With this new sample holder, the spectrophotometer exhibits enhanced detection sensitivity, especially at low concentrations.

Wed, Jul 30 10:30–12:30

ARCANE Reweighting: A technique to tackle the sign problem in the simulation of collider events in high energy physics

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Negatively weighted events, which appear in the Monte Carlo (MC) simulation of particle collisions, significantly increase the computational resource requirements of current and future collider experiments in high energy physics. This work introduces an MC technique called ARCANE reweighting for reducing or eliminating negatively weighted events. The technique works by redistributing (via an additive reweighting) the contributions of different pathways within the simulator that lead to the same final event. The technique is exact and does not introduce any biases in the distributions of physical observables. ARCANE reweighting can be thought of as a variant of the parametrized control variates technique, with the added nuance that redistribution is performed using a deferred additive reweighting. The technique is demonstrated for the simulation of a specific collision process, namely $e^+e^- \rightarrow q\bar{q} + 1\text{ jet}$. The technique can be extended to several other collision processes of interest as well. This talk is based on the Refs [1] and [2].

- [1] Shyamsundar, Prasanth (2025). *ARCANE Reweighting: A Monte Carlo Technique to Tackle the Negative Weights Problem in Collider Event Generation*. arXiv:2502.08052 [hep-ph].
- [2] Shyamsundar, Prasanth (2025). *A Demonstration of ARCANE Reweighting: Reducing the Sign Problem in the MC@NLO Generation of $e^+e^- \rightarrow q\bar{q} + 1\text{ jet}$ Events*. arXiv:2502.08052 [hep-ph].

Wed, Jul 30 10:30–12:30

Multifidelity and Surrogate Modeling Approaches for Uncertainty Quantification in Ice Sheet Simulations

Nicole Aretz

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Coauthor(s): Max Gunzburger, Mathieu Morlighem, Karen Willcox

Our work [1] uses multifidelity and surrogate modeling to achieve computationally tractable uncertainty quantification (UQ) for large-scale ice sheet simulations. UQ is of utmost importance to enable judicious policy decisions combating climate change. However, high-fidelity ice sheet models are typically too expensive computationally to permit Monte Carlo sampling. To reduce the computational cost while achieving the same target accuracy, we use multifidelity estimators to shift the computational burden onto less expensive surrogate models derived from coarser discretizations and approximated physics. In this talk, we compare three estimators — Multifidelity [2] and Multilevel [3] Monte Carlo, and the Best Linear Unbiased Estimator [4] — and present results for the expected ice mass loss of the Greenland ice sheet.

- [1] Aretz, N., Gunzburger, M., Morlighem, M., & Willcox, K. (2025). Multifidelity uncertainty quantification for ice sheet simulations. *Computational Geosciences*, 29(1), 1-22.
- [2] Peherstorfer, B., Willcox, K., & Gunzburger, M. (2016). Optimal model management for multifidelity Monte Carlo estimation. *SIAM Journal on Scientific Computing*, 38(5), A3163-A3194.
- [3] Giles, M. B. (2015). Multilevel monte carlo methods. *Acta numerica*, 24, 259-328.
- [4] Schaden, D., & Ullmann, E. (2020). On multilevel best linear unbiased estimators. *SIAM/ASA Journal on Uncertainty Quantification*, 8(2), 601-635.

Wed, Jul 30 14:00–16:00

Empirical Statistical Comparative Analysis of SNP Heritability Estimators and Gradient Boosting Machines (GBM) Using Genetic Data from the UK Biobank

Kazeem Adeleke^{*1}

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Coauthor(s): Peter Ogunyinka², Emmanuel Ologunleko³ and Dawud Agunbiade⁴

This study addresses the methodological challenges in estimating genetic heritability by

comparing traditional statistical approaches with advanced machine learning techniques. We evaluated three distinct methods: sibling regression, LD-score regression, and Gradient Boosting Machines (GBMs), using both simulated datasets and real-world data from the UK Biobank. Our methodology involved generating simulated genotypes following Mendelian inheritance patterns and creating corresponding phenotypes incorporating family-specific genetic effect sizes. We conducted Genome-Wide Association Studies (GWAS) on firstborn children from each family and performed comprehensive heritability analyses using all three methods. Results demonstrated that while sibling regression effectively captured within-family genetic similarities and LD-score regression accounted for population-wide linkage disequilibrium patterns, GBMs showed superior capability in predicting phenotypes by capturing complex genetic interactions. The integration of GBMs with traditional methods revealed enhanced predictive power and provided new insights into the genetic architecture of complex traits. Our findings emphasize the value of combining conventional statistical approaches with machine learning techniques for more robust heritability estimation in large-scale UK Biobank studies.

Wed, Jul 30 14:00–16:00

Cheap permutation testing

Carles Domingo-Enrich

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Coauthor(s): Raaz Dwivedi, Lester Mackey

Permutation tests are a popular choice for distinguishing distributions and testing independence, due to their exact, finite-sample control of false positives and their minimax optimality when paired with U-statistics. However, standard permutation tests are also expensive, requiring a test statistic to be computed hundreds or thousands of times to detect a separation between distributions. In this work, we offer a simple approach to accelerate testing: group your datapoints into bins and permute only those bins. For U and V-statistics, we prove that these cheap permutation tests have two remarkable properties. First, by storing appropriate sufficient statistics, a cheap test can be run in time comparable to evaluating a single test statistic. Second, cheap permutation power closely approximates standard permutation power. As a result, cheap tests inherit the exact false positive control and minimax optimality of standard permutation tests while running in a fraction of the time. We complement these findings with improved power guarantees for standard permutation testing and experiments demonstrating the benefits of cheap permutations over standard maximum mean discrepancy (MMD), Hilbert-Schmidt independence criterion (HSIC), random Fourier feature, Wilcoxon-Mann-Whitney, cross-MMD, and cross-HSIC tests.

Wed, Jul 30 14:00–16:00

Moving PCG beyond LCGs*Christopher Draper*

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Coauthor(s): Michael Mascagni

PCG is a set of generators released by Melissa E. O'Neill in 2014 [1]. The original technical report outlined a number of lightweight scrambling techniques. Each scrambling technique offered some improvement to the quality of the linear congruential generators they were designed for. However the real strength of the scrambling techniques was that they could easily be combined in different combinations to offer much stronger improvements. The PCG technical report concludes with the creation of the PCG library, a popular PRNG library that implements a number of generators described in the technical report. Starting from the observation that the PCG work was narrowly focused on implementing their scrambling techniques for specific linear congruential generators, we explore the PCG scrambling techniques and their potential application for being applied to other PRNGs. We show the steps taken to generalize the PCG scrambling techniques to work with any arbitrary amount of bits and parameter values. Then test the PCG scrambling techniques across different linear congruential generators and then test the PCG scrambling techniques across a number of different PRNGs.

- [1] Melissa E. O'Neill. 2014. PCG: A Family of Simple Fast Space-Efficient Statistically Good Algorithms for Random Number Generation. Technical Report HMC-CS-2014-0905. Harvey Mudd College, Claremont, CA.

Wed, Jul 30 14:00–16:00

Hybrid least squares for learning functions from highly noisy data*Yiming Xu*

University of Kentucky

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Coauthor(s): Ben Adcock, Bernhard Hientzsch, Akil Narayan

Motivated by the request for efficient estimation of conditional expectations, we consider a least-squares function approximation problem with heavily polluted data. In such scenarios, existing methods based on the small noise assumption become suboptimal. We propose a hybrid approach that combines Christoffel sampling with optimal experimental design to address this issue. The proposed algorithm adheres to appropriate optimality criteria for both

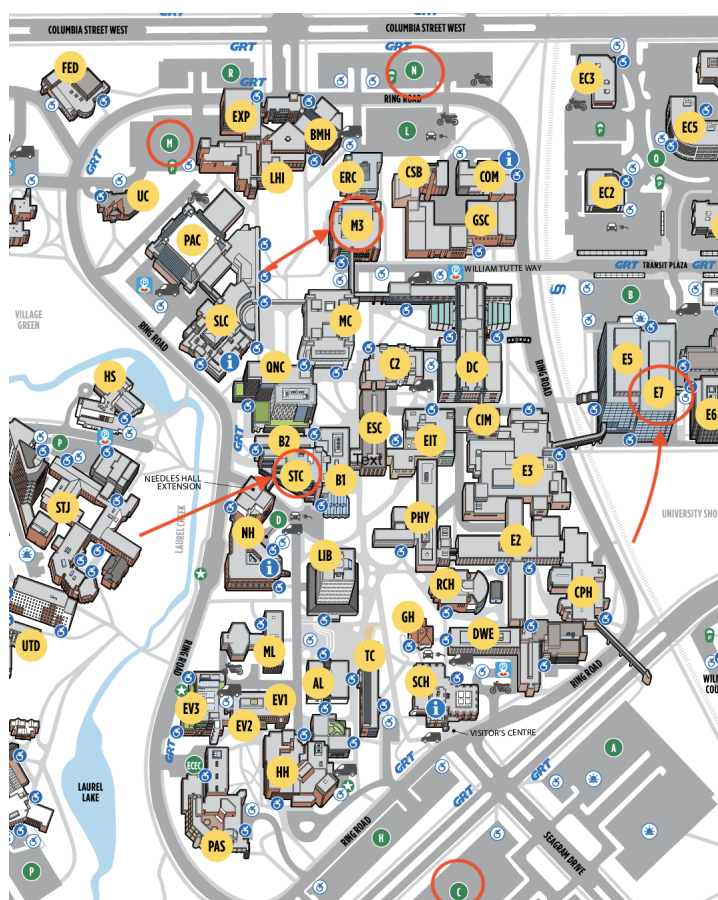
sample points generation and function evaluation, leading to improved computational efficiency and sample complexity. We also extend the algorithm to convex-constrained settings with similar theoretical guarantees. Moreover, when the target function is defined as the expectation of a random field, we introduce adaptive random subspaces to approximate the target function and establish results concerning its approximation capacity. Our findings are corroborated through numerical studies on synthetic data and a more challenging stochastic simulation problem in computational finance.

Practical Information

Location

The 16th edition of the MCQMC conference is hosted by the University of Waterloo. All talks will take place in the Science Teaching Complex (STC) in rooms STC 0020, STC 0040, STC 0050, STC 0060, which are located in the basement of STC, and also in STC 1012, which is located on the first floor.

The following shows a partial campus map where STC, Mathematics 3 (M3) and Engineering 7 (E7) are identified, the latter two being the venues for the Monday evening reception and Wednesday evening banquet, respectively. It also shows a few parking options (Lots C, M and N). A full campus map with building legend can be found [here](#).



Conference Schedule

The conference schedule included in this program book may not reflect last-minute changes to the schedule. The online version of the schedule on the conference website will be kept as much up-to-date as possible, reflecting also last minute changes.

Registration and Information Desk

The registration and information desk is located in the STC 1st floor foyer, outside of STC 1012. Sunday afternoon registration will take place from 13:30 to 16:00 on August 18. Monday (August 19) morning registration will take place from 08:00 to 12:30 and from 14:00

to 16:00 on. There will be support on site throughout the week for participants who arrive after Monday.

Sunday Tutorials

Sunday afternoon tutorials will be held in STC 1012, and are given by Fred Hickernell (14:15–15:45) and Peter Frazier (16:00–17:30).

Opening Ceremony

The opening ceremony will be held in STC 1012 on Monday, August 19, at 08:45, before the first plenary talk.

Plenary Talks

Plenary talks will be held in STC 1012. Plenary talks are 50 minutes long, plus 10 minutes for questions and discussions. Due to the tight conference schedule, we kindly ask the chairs to strictly observe the time constraints.

All other talks

All other talks (except plenary talks and tutorials) will be held in parallel sessions in STC 0020, STC 0040, STC 0050, and STC 0060. These talks are 25 minutes long plus 5 minutes for questions and discussions. Due to the tight conference schedule, we kindly ask all speakers and chairs to strictly observe the time constraints.

Coffee Breaks

Morning and afternoon coffee breaks will take place in the STC lower-level atrium, between the plenary talk and parallel sessions, i.e., from 10:00 to 10:30 and from 15:00 to 15:30. There will also be a coffee break on Sunday August 18 between the two tutorials, from 15:45 to 16:00.

Reception (Monday)

On Monday, August 19, there will be a welcome reception from 18:00 to 19:30. Drinks and finger food will be provided in the Mathematics 3 (M3) building atrium (ground floor). M3 is just north of the Mathematics & Computing (MC) building. Please refer to the conference website for campus maps or see above information on Location.

Award Ceremony of the Journal of Complexity (Monday)

On Monday, August 19, there will be a short ceremony to award IBC Awards and IBC Young Researcher Awards of the Journal of Complexity. The ceremony will be chaired by senior editors of the journal, and take place at about 8:55 in STC 1012 (immediately before the first plenary talk).

Conference Photo (Wednesday)

A conference photo will be taken on Wednesday, August 21, at 17:30, right after the afternoon parallel sessions. Details will be announced during the conference week.

Conference Dinner (Wednesday)

The conference dinner will take place in the Engineering 7 (E7) building, which is outside of Ring Road, immediately behind and directly connected from inside to the Engineering 5 (E5) building. You can find it easily as E5 is the building connected to campus by a bridge going over Ring Road near the Davis Centre.

Please note that all participants (conference participants and accompanying persons) must be registered in advance for this event.

Steering Committee Meeting (Thursday)

On Thursday, August 22, the MCQMC Steering Committee will have a closed meeting, starting at 19:00. If you have any comments or suggestions, or would like to propose hosting a future conference, please approach any member of the Steering Committee prior to this meeting.

Food

Lunch will *not* be provided. There will be a Tim Horton's (located in the Davis Centre (DC) ground floor), Subway and Flock Stop (both located in the Student Life Center - SLC ground floor), open on-campus during the week providing an inexpensive option for lunch. Alternatively, a short 10-minute walk east from STC leads to the "University Shops Plaza" where there are several restaurants and fast-food outlets providing more diverse options for conference participants. Another popular lunch venue is Ken Sushi House on Phillip Street, just east of campus.

Travel to Waterloo from Toronto Pearson Airport (YYZ)

Before you travel to Canada, please ensure you have the proper documents and visitor visas to visit. Check the Government of Canada website for specific requirements for your country.

Details regarding travel visas can be found on the registration page.

Waterloo is located approximately one hour by car from Toronto Pearson Airport, however there are several methods to book travel from the airport to Waterloo.

- By Bus: There are buses that travel between Toronto Pearson YYZ, to Waterloo. GO Transit is the most popular.
- By Taxi: With Waterloo Taxi, you can reserve a taxi on the Waterloo Taxi online form or call at +1 (519) 888-7777.
- By Rail: UP Express is a direct journey from Toronto Pearson International Airport to Union Station, Downtown Toronto. When at Union Station, transfer to VIA Rail train or GO train.
- By Airways Transit (up to 8 passengers): Reserve door-to-door service on the Airways Transit website. By Car: Take ON-401 W towards London and then take exit 278 to merge onto ON-8 W toward Kitchener/Waterloo.

Public transport in Waterloo

By Bus: Grand River Transit is the public transit operator for the Region of Waterloo, Ontario. It operates daily bus serves across Waterloo and the University of Waterloo campus.

By ION Light Rail Travel: ION is Waterloo Region's light rail transit (LRT) system. It runs between Kitchener's Fairview Park Mall and Waterloo's Conestoga Mall, with stops at the University of Waterloo campus. ION trains connect passengers to the existing bus system (Grand River Transit), making it easy to travel across the region.

Equipment in classrooms used for conference

Each lecture hall is equipped with a desktop computer running Windows, with USB port access and internet connection, a data projector and screen, and blackboards. One MCQMC staff member will be present in each lecture hall to assist with IT related issues.

We strongly encourage you to make yourself known to your session chair and (if necessary) the MCQMC staff member assigned to your lecture room, prior to your talk. Please prepare your talk in the form of a PDF or PPT document. A slides repository will be created shortly before the conference to facilitate the uploading of slides to the desktop computer in each room prior to each session by MCQMC staff. More detailed instructions will be sent to speakers and session chairs prior to the conference. An alternative option is to bring a USB storage device with your slides copied on it and make sure that your talk is copied onto the desktop computer during the break prior to your talk.

If you require access to other software packages or other audio-visual equipment, please communicate with the conference organizers well ahead of time to see if it can be arranged. It is possible to connect your personal laptop to the data projector, but we prefer that you avoid this option due to the tight conference schedule. If you need to use your own laptop, please make sure that you discuss this with a MCQMC staff member and that you test the connection well before your talk.

Internet and Computer Access

University of Waterloo has eduroam to provide free wireless access for visitors whose home institutions also have eduroam. For more information on eduroam see <http://www.eduroam.org>. Please check with your institution whether you have access to eduroam and for instructions on how to set up eduroam (this depends on your home institution and not on local institutions).

If you cannot use eduroam, conference participants will be granted access to the Waterloo wireless network on campus via self-registration. Further details on how to do so will be announced during the opening of the conference.

In any case, please use the wireless connections provided responsibly.

Emergency Contacts, Hospitals and Services on Campus

The emergency phone number in Canada is **911**. For emergency calls on-campus, call the UW Special Constable at 519-888-4911. There is a Special Constable on campus 24 hours a day, 7 days a week.

Local Kitchener-Waterloo Hospitals

- Grand River Hospital, 835 King Street West, Kitchener (519-742-3611)
- St. Mary's General Hospital, 911 Queen's Boulevard, Kitchener (519-744-3311)

Power Plugs in Canada

In Canada, the standard power sockets are:

- Type A:
 - Description: This socket has two flat parallel pins.
 - Voltage: 120 V
 - Frequency: 60 Hz
- Type B:
 - Description: This socket has two flat parallel pins and a grounding pin (three-pronged).
 - Voltage: 120 V
 - Frequency: 60 Hz

Closing of the Conference

MCQMC 2024 will be closed with a few short announcements and remarks immediately after the final parallel sessions, which finish at 12:30 on Friday, August 23.

Proceedings

Following the tradition of the MCQMC conference series, a selection of strictly refereed papers will be published after the conference as a Springer book. Every speaker is welcome to submit a paper based on his/her talk, with the length strictly not exceeding 16 pages in the Springer style. Plenary and tutorial speakers are invited to submit papers of at most 30 pages length. The papers of plenary and tutorial speakers can be survey articles.

The submission deadline for manuscripts is December 13, 2024. Please send your submissions as a pdf file to mcqmc.2024@uwaterloo.ca.

Further instructions will be provided in the closing session of the conference, and will be available on the conference website later.

Conference Statistics (as of July 5)

Number of participants	151
Number of plenary lectures	8
Number of tutorials	2
Number of talks	137
Number of special sessions	24 (85 talks)
Number of technical sessions	12 (42 talks)

List of Participants

FirstName LastName

Organization

p. ??

Christiane Lemieux

University of Waterloo

p. 22

Peter Glynn

Stanford University

p. 23

Roshan Joseph

Georgia Institute of Technology

p. 24

Michaela Szölgyenyi

University of Klagenfurt

p. 25

Uros Seljak

University of California, Berkeley

p. 26

Nicolas Chopin

ENSAE, Institut Polytechnique de Paris

p. 28

Stefan Heinrich

RPTU Kaiserslautern-Landau

p. 30

Chengcheng Ling

University of Augsburg

p. 30

Thomas Muller-Gronbach

University of Passau

p. 30

Andreas Neuenkirch

University of Mannheim

p. 30

Christopher Rauhogger

University of Passau

p. 30

Verena Schwarz

University of Klagenfurt

p. 30

Larisa Yaroslavtseva

University of Graz

p. 30

Murat Erdogdu

University of Toronto

p. ??

Sebastiano Grazzi

Bocconi University

p. ??

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KTH Royal Institute of Technology

p. ??

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Queen Mary University of London

p. ??

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University of Amsterdam

p. ??

Jun Yang

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p. ??

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p. ??

Sou-Cheng Choi

Illinois Institute of Technology

p. ??

Yuhan Ding

Illinois Institute of Technology

p. ??

Hwanwoo Kim

Duke University

p. ??

Michael Mascagni
Florida State University
p. ??

Jonathan Weare
New York University
p. ??

Stefan Heinrich
RPTU Kaiserslautern-Landau
p. 34

Andre Herzwurm
Rosenheim Technical University of Applied
Sciences
p. 34

Gunther Leobacher
University of Graz
p. 34

Thomas Muller-Gronbach
University of Passau
p. 34

Alexander Steinecke
University of Leoben
p. 34

Larisa Yaroslavtseva
University of Graz
p. 34

Alen Alexanderian
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p. ??

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p. ??

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Inria
p. ??

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p. ??

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p. ??

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p. ??

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p. ??

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p. ??

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p. ??

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p. ??

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p. ??

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p. ??

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p. ??

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Fermilab
p. ??

Ziang Niu
University of Pennsylvania
p. ??

Chenyang Zhong
Columbia University
p. ??

Stefan Heinrich
RPTU Kaiserslautern-Landau
p. 35

Bernd Kaßemodel
Chemnitz University of Technology
p. 35

Thomas Muller-Gronbach
University of Passau
p. 35

Klaus Ritter
RPTU Kaiserslautern-Landau
p. 35

Matti Vihola
University of Jyväskylä
p. 35

Larisa Yaroslavtseva
University of Graz
p. 35

Chaofan Huang
Georgia Institute of Technology
p. ??

Lulu Kang
University of Massachusetts Amherst
p. ??

Chunfang Lin
Queen's University
p. ??

Simon Mak
Duke University
p. ??

Chih-Li Sung
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p. ??

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Shanghai Jiao Tong University
p. ??

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p. ??

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p. ??

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p. ??

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New York University
p. ??

Art Owen
Stanford University
p. ??

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p. ??

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Cornell University
p. ??

Raghu Pasupathy
Purdue University
p. ??

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p. ??

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p. ??

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p. ??

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p. ??

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p. ??

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p. ??

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p. ??

Aleksandar Nikolov
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p. ??

Peng Zhang
Rutgers University
p. ??

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p. ??

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Florida State University
p. ??

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Florida State University and National
Institute of Standards and Technology
p. ??

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Nvidia Corporation
p. ??

Silei Song
Florida State University
p. ??

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p. ??

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p. ??

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p. ??

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p. ??

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p. ??

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p. ??

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p. ??

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p. ??

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New York University
p. ??

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p. ??

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p. ??

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p. ??

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p. ??

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Technology/RWTH Aachen University
p. 36

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p. 36

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and Applied Mathematics
p. 36

Zhijian He
South China University of Technology
p. 36

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p. 36

Michael Gnewuch
University of Osnabrück
p. ??

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p. ??

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p. ??

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p. ??

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p. ??

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p. ??

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p. ??

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p. ??

Xiaoou Cheng
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p. ??

Siddharth Mitra
Yale University
p. ??

Molei Tao
Georgia Institute of Technology
p. ??

Jonathan Weare
New York University
p. ??

Jose Blanchet
Stanford University
p. 37

Jing Dong
Columbia University
p. 37

Chang-Han Rhee

Northwestern University
p. 37

Maksim Chupin

King Abdullah University of Science and
Technology
p. 38

Zhou Fang

Chinese Academy of Sciences
p. 38

Chiheb Ben Hammouda

Utrecht University
p. 38

Sophia Munker

RWTH Aachen University
p. 38

Muruhan Rathinam

University of Maryland, Baltimore
p. 38

Raul Tempone

RWTH Aachen University
p. 38

Niklas Baumgarten

University of Heidelberg
p. ??

Sou-Cheng Choi

Illinois Institute of Technology
p. ??

Joseph Farmer

University of Notre Dame
p. ??

Mike Giles

University of Oxford
p. ??

Johannes Krotz

University of Notre Dame
p. ??

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p. ??

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p. ??

Arved Bartuska

King Abdullah University of Science and
Technology/RWTH Aachen University
p. 31

Truong Vinh Hoang

RWTH Aachen University
p. 31

Vesa Kaarnioja

Free University of Berlin
p. 31

Sebastian Krumscheid

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p. 31

Raúl Tempone

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Technology/RWTH Aachen University
p. 31

Sou-Cheng Choi

Illinois Institute of Technology
p. ??

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p. ??

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p. ??

Chung Ming Loi

Durham University
p. ??

Pieterjan Robbe

Sandia National Laboratories
p. ??

Michael Gnewuch

Osnabruck University
p. 32

Stefan Heinrich

RPTU Kaiserslautern-Landau
p. 32

Thomas Muller-Gronbach

University of Passau
p. 32

Leszek Plaskota

University of Warsaw
p. 32

Kateryna Pozharska

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p. 32

Marcin Wnuk

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p. 32

Larisa Yaroslavtseva

University of Graz
p. 32

Arved Bartuska

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p. ??

Philipp A. Guth

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p. ??

Tapio Helin

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p. ??

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p. ??

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p. ??

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p. ??

Makram Chahine

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p. ??

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p. ??

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p. ??

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p. ??

Jean-Francois Chassagneux

ENSAE Paris
p. 33

Goncalo Dos Reis

University of Edinburgh
p. 33

Noufel Frikha

Paris 1 Pantheon-Sorbonne University
p. 33

Stefan Heinrich

RPTU Kaiserslautern-Landau
p. 33

Thomas Muller-Gronbach

University of Passau
p. 33

Sotirios Sabanis

University of Edinburgh
p. 33

Larisa Yaroslavtseva
University of Graz
p. 33

Ayoub Belhadji
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p. ??

Adrien Corenflos
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p. ??

Florence Forbes
Inria
p. ??

Xun Huan
University of Michigan
p. ??

Youssef Marzouk
Massachusetts Institute of Technology
p. ??

Zhihao Wang
University of Copenhagen
p. 59

Ruben Seyer
Chalmers University of Technology and
University of Gothenburg
p. 60

Philippe Gagnon
Université de Montréal
p. 61

Attila Lovas
Hun-Ren Alfréd Rényi Institute of
Mathematics
p. 85

Iosif Lytras
Athena Research Centre
p. 86

Sara Pérez-Vieites
Aalto University
p. 87

Nikolaos Makras
University of Edinburgh
p. 88

Fabio Zoccolan
EPFL
p. 88

Anke Wiese
Heriot-Watt University
p. 89

Riccardo Saporiti
EPFL
p. 90

Leon Wilkosz
King Abdullah University of Science and
Technology
p. 91

Adrien Richou
Université de Bordeaux
p. 92

Abdujabar Rasulov
University of World Economy and
Diplomacy
p. 92

Miguel Alvarez
King Abdullah University of Science and
Technology
p. 93

Håkon Hoel
University of Oslo
p. 94

Frédéric Blondeel
Kuleuven and Unife
p. 95

Du Ouyang
Tsinghua University
p. 95

Wei Cai
Southern Methodist University
p. 96

Yiqing Zhou
KU Leuven
p. 97

Kevin Bitterlich
TU Bergakademie Freiberg
p. 97

Reuben Cohn-Gordon
University of California, Berkeley
p. 98

Philip Schaer
Friedrich Schiller University Jena
p. 99

Annabelle Carrell
University of Cambridge
p. 100

Philippe Blondeel
Belgian Military Academy
p. 100

Rino Persiani
INFN Catania
p. 101

Prasanth Shyamsundar
Fermi National Accelerator Laboratory
p. 102

Nicole Aretz
University of Texas at Austin
p. 103

Kazeem Adeleke
University of the West of England
p. 103

Carles Domingo-Enrich
Microsoft Research New England
p. 104

Christopher Draper
Florida State University
p. 105

Yiming Xu
University of Kentucky
p. 105

Lorenzo Nagar
Basque Center for Applied Mathematics
p. 62

Hamza Ruzayqat
King Abdullah University of Science and
Technology
p. 63

Arghya Datta
Université de Montréal
p. 64

Jimmy Lederman
University of Chicago
p. 64

Yashveer Kumar
INESC-ID
p. 66

Serena Fattori
Istituto Nazionale di Fisica Nucleare
(INFN)
p. 66

Toon Ingelaere
KU Leuven
p. 68

Muhammad Noor ul Amin
COMSATS University Islamabad, Lahore
p. 68

Christian Weiss

Ruhr West University of Applied Sciences
p. 69

Xiaoda Xu

Suqian University
p. 69

Sifan Liu

Flatiron Institute
p. 70

Ambrose Emmett-Iwaniw

University of Waterloo
p. 70

Peter Kritzer

Austrian Academy of Sciences
p. 71

Yang Liu

King Abdullah University of Science and
Technology
p. 72

Jakob Dilen

KU Leuven
p. 73

Aadit Jain

Rancho Bernardo High School
p. 73

Akash Sharma

Chalmers Institute of Technology
p. 74

Joonha Park

University of Kansas
p. 75

Arne Bouillon

KU Leuven
p. 76

Alex Shkolnik

University of California, Santa Barbara
p. 76

Kun-Lin Kuo

National University of Kaohsiung
p. 77

Sascha Holl

Max Planck Institute for Informatics
p. 77

Josephine Westermann

Heidelberg University
p. 79

Soumyadip Ghosh

IBM Research
p. 79

Matyokub Bakoev

MGIMO, Tashkent
p. 80

Vincent Zhang

University of Southern California
p. 81

Hao Quan

University of Waterloo
p. 83

Nicola Branchini

University of Edinburgh
p. 83

Daniel Yukimura

Impa, Rio de Janeiro
p. 84

Amit Subrahmanya

Virginia Tech
p. 85

André Gustavo Carlson

RWTH Aachen University

Noufel Frikha

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