



Welcome to MCQMC2026!

We are delighted to welcome you to Edinburgh for the *17th International Conference on Monte Carlo and Quasi-Monte Carlo Methods in Scientific Computing* (MCQMC). The MCQMC conference series is, together with its sister conference series on Monte Carlo Methods (MCM), a major event for researchers in the Monte Carlo and quasi-Monte Carlo communities. We are glad to host MCQMC in Scotland for the first time and in the United Kingdom for a second time, the first being in Oxford (2020).

MCQMC2024 marked the thirty-year anniversary of the first MCQMC conference held in 1994, and the event was commemorated with a panel discussion on the vibrant current research community, significant past achievements and milestones, and exciting future challenges. MCQMC2026 yet again confirms the research activity and interest in Monte Carlo and quasi-Monte Carlo methods and related fields in efficient approximation and inference, and features 230 participants from 24 countries, 7 plenary talks, 2 tutorials, 25 special sessions, and 53 contributed talks. The speakers come from a variety of scientific backgrounds, countries, institutions and career stages.

Founded in 1583, the University of Edinburgh is one of the largest universities in Scotland with around 50 000 students. The Maxwell Institute, which brings together the School of Mathematics at the University of Edinburgh and the School of Mathematical and Computer Sciences at Heriot-Watt University, hosts strong local research groups in several areas central to MCQMC, including multilevel Monte Carlo methods, Markov chain Monte Carlo methods, sequential Monte Carlo methods, Monte Carlo methods in SDEs and SPDEs, kernel methods and scientific machine learning for sampling.

Being the capital city of Scotland, Edinburgh offers cultural and historical richness. It is a renowned city for arts, with the *old town* a UNESCO World Heritage Site and the city a UNESCO City of Literature. Edinburgh also hosts the worlds largest arts festival, the Fringe Festival, which occurs every year! We hope you enjoy your stay in this great city, and may you leave with as many stories as its centuries-old streets have to tell.

We wish you a productive and interesting week at MCQMC2026!

Neil Chada, Abdul-Lateef Haji-Ali, Chris Oates, Aretha Teckentrup, Sara Wade, Konstantinos Zygalakis

MCQMC2026 Conference Organizers

May 20th, 2026

Conference website: <https://maths.ed.ac.uk/events/mcqm-2026>

About MCQMC

History

The MCQMC conference is a biennial meeting bringing together scholars engaged in Monte Carlo and Quasi Monte Carlo methods and closely related fields. The conference focuses primarily on the mathematical study of these techniques, their implementation and adaptation for concrete applications, and their empirical assessment. Its aim is to provide a forum where leading researchers and users can exchange information on the latest theoretical developments as well as important applications of these methods.

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

The previous instances of MCQMC 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),
16. Waterloo, Canada (2024).

Steering Committee

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Wales, Australia)
Takashi Goda (The University of Tokyo,
Japan)
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Technology, USA)
Alexander Keller (NVIDIA, Chair)

Peter Kritzer (RICAM, Austria)
Christiane Lemieux (University of
Waterloo, Canada)
Art Owen (Stanford University, USA)
Aretha Teckentrup (University of
Edinburgh, UK)

Topics

- Monte Carlo, variance reduction methods
- Multilevel Monte Carlo
- quasi-Monte Carlo, randomised quasi-Monte Carlo
- Digital nets and lattice rules
- Discrepancy theory
- Complexity and tractability of multivariate problems
- Kernel methods, high-dimensional approximation
- Markov chain Monte Carlo
- Sequential Monte Carlo
- Gradient flows and machine learning for sampling
- Rare event simulation
- Software for MC/QMC, probabilistic programming
- MC/QMC methods in physics, chemistry, finance, computer graphics, machine learning, and other areas

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- Sebastian Reich (University of Potsdam, Germany)
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- Abdul-Lateef Haji-Ali (Heriot-Watt University)
- Jonas Latz (University of Manchester)
- Chris Oates (Newcastle University)
- Aretha Teckentrup (University of Edinburgh) - Head of committee
- Sara Wade (University of Edinburgh)
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MAC-MIGS Centre for Doctoral Training

<https://www.mac-migs.ac.uk/>

ProbAI hub

<https://www.probai.uk>



Conference Location

MCQMC2026 will take place on the King's Buildings campus of the University of Edinburgh. The campus is easily accessible by bus from around the city: services 9 (stop King's Buildings, final stop), 12 and 24 (stop Rankin Drive), 38 (stop West Mains Road), and 3, 7, 8, 29, 31, 37 and 47 (stop Lady Road) all stop within a 5-10 minute walk of the conference venue.

We will use the Michael Swann, James Clerk Maxwell and Nucleus buildings for the conference.

Michael Swann Building (Swann)

- **Main Lecture Theatre:** This room will be used for **tutorials and plenary talks**. The entrance is on the ground floor of the Swann building, immediately to the right after the main entrance.

James Clerk Maxwell Building (JCMB)

- **Lecture Theatres A, B, C:** These rooms will be used for **special sessions and contributed talks**. The entrance is from level 2 (ground floor) or level 3 of JCMB, immediately to the left at the main entrance (level 2) or the Magnet Café (level 3).
- **Rooms 5326, 5327, 5238:** These rooms will be used for **special sessions and contributed talks**. The entrance is from level 5 of JCMB, behind the main lifts.
- **Room 6206:** This room will be used for **special sessions and contributed talks**. The entrance is from level 6 of JCMB, down the 62 corridor to the left from the main lifts.
- **Rooms 3211, 3217:** These rooms can be used for **working space or meetings by participants**. The entrance is from level 3 of JCMB, close to the Magnet Café.
- **Rooms 5205:** This room can be used for **working space or meetings by participants**. The entrance is from level 5 of JCMB, down the 52 corridor to the left from the main lifts.
- **Magnet Café:** This space will be used for all **coffee and lunch breaks** during the conference. It is located on level 3 of JCMB. To reach this space, go one floor up from the main entrance.

Nucleus Building

- **Second Floor Foyer and Balcony:** This space will be used for the **drinks reception** on Monday evening. To reach this space, go one floor up from the main entrance.

Special Thanks

The conference organizers would like to thank all sponsors for making this event possible, and the University of Edinburgh for providing us with the space needed to host this conference. We are incredibly grateful for the organizational support from Katie Green in the School of Mathematics at the University of Edinburgh and Alex Liu from the International Centre for Mathematical Sciences, without whom this conference would not have run as smoothly. We are indebted to the generous support and advice from past MCQMC conference organizers Christiane Lemieux and Nathan Kirk. The conference chair, Aretha Teckentrup, is grateful to the local organizing committee for all their help.

We further wish to extend our thanks to the Steering Committee for giving us the opportunity to host this conference and for sharing their expertise with us, and to the Scientific Committee for their valued input to the scientific programme. We thank our plenary speakers, tutorial speakers, special session organizers, and all session chairs for their help and support with the scientific organization of the conference.

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Schedule

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10:00–10:30		Coffee break	Coffee break	Coffee break	Coffee break
10:30–11:00	Coffee break	Parallel sessions II	Parallel sessions IV	Parallel sessions V	Parallel sessions VII
11:00–12:30	Tutorial: Lemieux (11.15am-12.45pm)				
12:30–14:00	Lunch break				
14:00–15:00	Plenary: Lang	Plenary: Alquier	Free afternoon	Plenary: Rhee	Free afternoon
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15:30–17:30	Parallel sessions I	Parallel sessions III		Parallel sessions VI	
17:30–	Drinks reception				
18:00–			Conference dinner		

Monday June 8th – Morning

08:30 – 17:00	Registration (JCMB Foyer)
09:00 – 09:15	Opening Remarks (Swann Main Lecture Theatre)
09:15 – 10:45	Swann Main Lecture Theatre Tutorial (TU01) <i>Victor Elvira</i> “A Primer on Importance Sampling and Particle Filters” p. 29 Chair: <i>Aretha Teckentrup</i>
10:45 – 11:15	Coffee Break (JCMB Magnet Café)
11:15 – 12:45	Swann Main Lecture Theatre Tutorial (TU02) <i>Christiane Lemieux</i> “Introduction to Quasi-Monte Carlo” p. 29 Chair: <i>Aretha Teckentrup</i>
12:45 – 14:00	Lunch Break (JCMB Magnet Café, 3217, 3211)

Monday June 8th – Afternoon/1

14:00 – 15:00	Swann Main Lecture Theatre Plenary Talk (PT01) <i>Annika Lang</i> “Random fields and stochastic partial differential equations on hypersurfaces” p. 31 Chair: <i>Sara Wade</i>			
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14:00 – 15:00	Swann Main Lecture Theatre Plenary Talk (PT01) <i>Annika Lang</i> “Random fields and stochastic partial differential equations on hypersurfaces” p. 31 Chair: <i>Sara Wade</i>		
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Tuesday June 9th – Morning/2

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Tuesday June 9th – Afternoon/1

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Tuesday June 9th – Afternoon/2

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Wednesday June 10th – 1

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11:00 – 11:30	<i>Lukasz Stepien</i> Exact asymptotic error and optimality of adaptive Milstein scheme for global approximation of SDEs with countably dimensional noise p. 103	<i>Hanyue Gu</i> Multimodal Laplace-based sampling p. 104	<i>Philipp Wacker</i> An optimal experimental design approach to sensor placement in continuous stochastic filtering p. 104	<i>Louise Kluge</i> Hierarchical Delayed Acceptance using Gaussian Process Surrogates p. 105
11:30 – 12:00	<i>Larisa Yaroslavtseva</i> On lower error bounds for strong approximation of SDEs with Hölder continuous drift coefficient p. 106	<i>Anya Katsevich</i> High-dimensional Laplace asymptotics up to the concentration threshold p. 107	<i>Lisa Hickl</i> On the Algorithmic and Theoretical Path Towards Optimal Personalised Treatment p. 107	<i>Leon Wilkosz</i> Stochastic Optimal Control for a System of Delay Equations arising from Heat and Humidity Control p. 108
12:00 – 12:30	<i>Nikolaos Makras</i> The Tamed Subgradient Unadjusted Langevin Algorithm beyond Convexity p. 108	<i>Dana Wrischnig</i> Wasserstein Stability of Bayesian Posteriors in the Concentrated Posterior Regime p. 109	<i>Joël Tatang Demano</i> Piecewise Deterministic Sampling for Constrained Distributions p. 109	<i>Riccardo Saporiti</i> Multilevel Markov chain Monte Carlo for a class of partially observed diffusions with noiseless observations p. 110
12:30 – 14:00	Lunch Break (JCMB Magnet Café, 3217, 3211)			
14:00 – 18:00	Free Afternoon			
18:00	Conference dinner (National Museum of Scotland)			

Wednesday June 10th – 2

09:00 – 09:05	Journal of Complexity Best Paper Award Ceremony		
09:05 – 10:00	Swann Main Lecture Theatre Plenary Talk (PT04) <i>Fred J. Hickernell</i> “Where Quasi-Monte Carlo Theory and Practice Meet” p. 32 Chair: <i>Abdul-Lateef Haji-Ali</i>		
10:00 – 10:30	Coffee Break (JCMB Magnet Café)		
10:30 – 12:30	JCMB 5327 Special Session (SS20) Sample Points: Quality Measures, Constructions, and Applications p. 49 Chair: <i>Michael Gnewuch</i>	JCMB 5328 Special Session (SS07) MLMC for SPDEs p. 50 Chair: <i>Mike Giles</i>	JCMB 6206 Technical Session (CT05) Rare Events Chair: <i>Marie Temple-Boyer</i>
10:30 – 11:00	<i>Dmitriy Bilyk</i> Energies with Tensor Product Structure, Fibonacci Lattices, and One-Distance Sets on the Torus p. 111	<i>Abdul-Lateef Haji-Ali</i> Hierarchical Methods for Semilinear Stochastic Partial Differential Equations p. 111	<i>Marie Temple-Boyer</i> Decision-making on a critical system using a rare event splitting technique p. 112
11:00 – 11:30	<i>Yoshihito Kazashi</i> Optimality of quasi-Monte Carlo methods and suboptimality of the sparse-grid Gauss–Hermite rule p. 114	<i>Annika Lang</i> Sampling the “same” coloured noise on different grid levels p. 115	<i>Jun Cheng</i> Sequentially Adaptive Emulators for Rare Event Estimation p. 115
11:30 – 12:00	<i>Dirk Nuyens</i> Multi-fidelity quasi-Monte Carlo p. 115	<i>Mike Giles</i> Different MLMC treatments of the stochastic heat equation p. 116	<i>Huiyi Chen</i> Wasserstein Distributionally Robust Rare-Event Simulation p. 116
12:00 – 12:30	<i>Ian H. Sloan</i> Doubling the convergence rate with kernel approximation p. 117		<i>Koen De Turck</i> Rare-Event Simulation of Top- k Exclusion in Mean-Field Elo Rating Models p. 117
12:30 – 14:00	Lunch Break (JCMB Magnet Café, 3217, 3211)		
14:00 – 18:00	Free Afternoon		
18:00	Conference dinner (National Museum of Scotland)		

Thursday June 11th – Morning/1

09:00 – 10:00	Swann Main Lecture Theatre Plenary Talk (PT05) <i>Kateryna Pozharska</i> “How to recover a function: optimal methods and theoretical guarantees” p. 33 Chair: <i>Aretha Teckentrup</i>			
10:00 – 10:30	Coffee Break (JCMB Magnet Café)			
10:30 – 12:30	JCMB Lecture Theatre A Special Session (SS25) Complexity of high-dimensional approximation p. 51 Chair: <i>Peter Kritzer</i>	JCMB Lecture Theatre B Special Session (SS19-1) New developments in quasi-Monte Carlo methods, Part 1 p. 51 Chair: <i>Zexin Pan</i>	JCMB Lecture Theatre C Special Session (SS16) Probabilistic couplings for the design and analysis of Monte Carlo methods p. 52 Chair: <i>Shiva Darshan</i>	JCMB 5326 Special Session (SS21) Practical aspects of Monte Carlo simulation in applications p. 53 Chair: <i>Emil Løvbak</i>
10:30 – 11:00	<i>Erich Novak</i> Numerical Integration and its Complexity for Functions with Uniformly Bounded Derivatives p. 118	<i>Josef Dick</i> The star discrepancy of a union of randomly digitally shifted Korobov (polynomial) lattice point sets depends polynomially on the dimension p. 118	<i>Adrien Corenflos</i> Computing importance weights for Markov chain Monte Carlo via couplings: an application to f-divergence diagnostics p. 119	<i>Sidney Hansen</i> Rendering volumes with bitmasks p. 119
11:00 – 11:30	<i>Yuya Suzuki</i> Approximation of differential entropy in Bayesian optimal experimental design p. 120	<i>Takashi Goda</i> Space-filling lattice designs for computer experiments p. 120	<i>Peter A. Whalley</i> Scalable Langevin Monte Carlo Methods for Bayesian Inference p. 121	<i>Thijs Steel</i> Artificially reduced collisionality Monte Carlo, an approximation method for neutral particles in the plasma edge of a fusion reactor p. 122
11:30 – 12:00	<i>Moritz Moeller</i> Instance optimal sampling recovery and minimal number of samples p. 122	<i>Du Ouyang</i> Quasi-Monte Carlo for SDE Simulation: Error Analysis and Dimensionality Reduction p. 123	<i>Tamás P. Papp</i> Scaling couplings of Markov chain Monte Carlo algorithms to high dimensions p. 123	<i>Dániel Hajnal</i> Multifidelity Uncertainty Quantification for Photon Radiotherapy p. 124
12:00 – 12:30	<i>Peter Kritzer</i> L_2 -approximation using median lattice algorithms p. 125	<i>Jianlong Chen</i> Convergence Analysis for Generative Models with Quasi-Monte Carlo Importance Sampling p. 125	<i>Joona Karjalainen</i> Mixing time of the conditional backward sampling particle filter p. 126	<i>Caleb Sbani</i> Reversing SPRNG: on Reversible Pseudorandom Number Generators p. 126
12:30 – 14:00	Lunch Break (JCMB Magnet Café, 3217, 3211)			

Thursday June 11th – Morning/2

09:00 – 10:00	Swann Main Lecture Theatre Plenary Talk (PT05) <i>Kateryna Pozharska</i> “How to recover a function: optimal methods and theoretical guarantees” p. 33 Chair: <i>Aretha Teckentrup</i>		
10:00 – 10:30	Coffee Break (JCMB Magnet Café)		
10:30 – 12:30	JCMB 5327 Special Session (SS22) Recent Advances in Gibbs Sampling p. 54 Chair: <i>Andi Q. Wang</i>	JCMB 5328 Technical Session (CT06) Markov chains and Monte Carlo Chair: <i>Mareike Hasenpflug</i>	JCMB 6206 Technical Session (CT07) Multilevel Methods and PDEs Chair: <i>Paul Mycek</i>
10:30 – 11:00	<i>Mengxi Gao</i> Weak Poincaré inequalities for Deterministic-scan Metropolis-within-Gibbs samplers p. 127	<i>Mareike Hasenpflug</i> Wasserstein de-initialization for Markov chains p. 127	<i>Paul Mycek</i> A filtered multilevel Monte Carlo method for the normalization of diffusion-based covariance operators p. 128
11:00 – 11:30	<i>Qian Qin</i> On spectral decomposition for Markov chains p. 129	<i>Julian Hofstadler</i> Solving Poisson’s equation for Wasserstein contractive Markov chains p. 129	<i>Toon Ingelaere</i> Single-ensemble multilevel simulation of McKean-Vlasov equations p. 129
11:30 – 12:00	<i>Cecilia Secchi</i> Spectral gap of Metropolis-within-Gibbs under log-concavity p. 130	<i>El Mahdi Khribch</i> On Monte Carlo with Global Proposals p. 130	<i>Wenhui (Joanna) Ni</i> Coarse-to-Fine Coupling for Accelerated Probabilistic Shape Modelling p. 131
12:00 – 12:30		<i>Aadit Jain</i> RQMC for Confidence Intervals using a Bounded Kurtosis Assumption p. 132	<i>Vesa Kaarnioja</i> Gevrey class and beyond in PDE uncertainty quantification p. 133
12:30 – 14:00	Lunch Break (JCMB Magnet Café, 3217, 3211)		

Thursday June 11th – Afternoon/1

14:00 – 15:00	Swann Main Lecture Theatre Plenary Talk (PT06) <i>Chang-Han Rhee</i> “Stochastic Simulation Perspectives on AI: Global Dynamics of SGD and Average-Reward Reinforcement Learning” p. 33 Chair: <i>Neil Chada</i>		
15:00 – 15:30	Coffee Break (JCMB Magnet Café)		
15:30 – 17:30	JCMB Lecture Theatre A Special Session (SS01-5) Stochastic computation and complexity, Part 6 p. 54 Chair: <i>Stefan Heinrich</i>	JCMB Lecture Theatre B Special Session (SS19-2) New developments in quasi-Monte Carlo methods, Part 2 p. 55 Chair: <i>Zexin Pan</i>	JCMB Lecture Theatre C Special Session (SS17) Bayesian inference using Monte Carlo and quasi-Monte Carlo methods p. 55 Chair: <i>Vesa Kaarnioja</i>
15:30 – 16:00	<i>Fred J. Hickernell</i> Good Lattice and Kronecker Sequences for Arbitrary Sample Size p. 133	<i>Yu Xu</i> Nested Multilevel Monte Carlo with Preintegration for Efficient Risk Estimation p. 134	<i>Laura Scarabosio</i> High-Dimensional Bayesian Level Set Inversion in Time-Domain Acoustic Waves p. 134
16:00 – 16:30	<i>Daniel Rudolf</i> Gibbsian polar slice sampling p. 135	<i>Yang Liu</i> Quasi-Monte Carlo with a Hankel random digital net p. 135	<i>Max Orteu Capdevila</i> Fast Bayesian shape parameter estimation for parabolic PDEs in moving domains p. 136
16:30 – 17:00	<i>Michael Gnewuch</i> Optimality of QMC Quadrature Rules on Multiple Scales of Function Spaces p. 136	<i>Valerie Ho</i> Randomized Quasi-Monte Carlo for Walk on Spheres p. 137	<i>Philipp A. Guth</i> Bayesian inference for output-feedback control of uncertain linear systems p. 138
17:00 – 17:30	<i>Leszek Plaskota</i> Optimal approximation of piecewise smooth functions from information contaminated with random noise p. 138		<i>Charlotte Lämberg</i> A Novel Convolutional Path Approach for Sampling with Interacting Particle Systems p. 139

Thursday June 11th – Afternoon/2

14:00 – 15:00	Swann Main Lecture Theatre Plenary Talk (PT06) <i>Chang-Han Rhee</i> “Stochastic Simulation Perspectives on AI: Global Dynamics of SGD and Average-Reward Reinforcement Learning” p. 33 Chair: <i>Neil Chada</i>		
15:00 – 15:30	Coffee Break (JCMB Magnet Café)		
15:30 – 17:30	JCMB 5326 Technical Session (CT08) Applications Chair: <i>Philippe Blondeel</i>	JCMB 5327 Technical Session (CT10) Sampling Chair: <i>Giorgos Vasdekis</i>	JCMB 5328 Technical Session (CT13) SDEs and Finance Chair: <i>Anke Wiese</i>
15:30 – 16:00	<i>Philippe Blondeel</i> Further investigations of the use of quasi-Monte Carlo in a Stochastic Optimal Control Framework for Maritime Mine Countermeasure Simulations p. 140	<i>Giorgos Vasdekis</i> Skew-symmetric schemes for robust SDE sampling. p. 141	<i>Anke Wiese</i> A Chen-Strichartz series expansion for Lévy models p. 141
16:00 – 16:30	<i>Veronika Chronholm</i> Uncertainty Quantification in Stochastic Modelling of Proton Beam Therapy p. 142	<i>Han Chen</i> Diffusion-Guided Proposals for Efficient High-Dimensional MCMC p. 142	<i>Tim Johnston</i> Numerical Methods for Singular SDEs p. 143
16:30 – 17:00	<i>Stephanie Schwab</i> Uncertainty Quantification in Cloud Physics p. 143	<i>Emil Løvbak</i> Metropolis-Hastings Acceptance Behavior for Bayesian Inversion with Random Forward Solvers p. 144	<i>Onni Hinkkanen</i> Quantitative discrete time hedging under initial insider information p. 145
17:00 – 17:30	<i>Callum Macaulay</i> Integrated Monte Carlo Pipeline for Emulation and Inference in a Biomechanical Arterial Model p. 145	<i>Nicola Branchini</i> Adaptively Learning the Optimal Proposal for Self-Normalized Importance Sampling p. 146	<i>Haitao Wang</i> Randomised Euler-Maruyama method for SDEs with Hölder continuous drift coefficient driven by α -stable Lévy process p. 146

Friday June 12th

09:00 – 10:00	Swann Main Lecture Theatre Plenary Talk (PT07) <i>Marylou Gabrié</i> “Assisting sampling of physical systems and Bayesian Inference with generative models” p. 34 Chair: <i>Jonas Latz</i>			
10:00 – 10:30	Coffee Break (JCMB Magnet Café)			
10:30 – 12:30	JCMB Lecture Theatre A Special Session (SS01-6) Stochastic computation and complexity, Part 5 p. 56 Chair: <i>Stefan Heinrich</i>	JCMB Lecture Theatre B Special Session (SS24) MCQMC for digital twins p. 56 Chair: <i>Philipp A. Guth</i>	JCMB Lecture Theatre C Special Session (SS23-2) Recent advances in hierarchical methods for uncertainty quantification, Part 2 p. 57 Chair: <i>Arved Bartuska</i>	JCMB 5326 Special Session (SS18) Monte Carlo Methods for Stochastic Reaction Networks p. 58 Chair: <i>Chiheb Ben Hammouda</i>
10:30 – 11:00	<i>David Krieg</i> A construction for optimal least squares approximation p. 147	<i>Frances Y. Kuo</i> Quasi-Monte Carlo for precision oncology – towards predictive digital twins p. 147	<i>Arved Bartuska</i> Multilevel double-loop quasi-Monte Carlo methods for nested integration p. 148	<i>David J. Warne</i> Multifidelity simulation and inference methods for non-Markovian reaction networks p. 149
11:00 – 11:30	<i>Kateryna Pozharska</i> Function discretization and related questions p. 149	<i>Tapio Helin</i> Efficient Entropy-Driven Strategies for Bayesian Optimal Experimental Design p. 150	<i>Matteo Raviola</i> A function approximation algorithm using multilevel active subspaces p. 150	<i>Juan David Marmolejo Lozano</i> Effects of Model Reduction on Coherence and Information Transfer in Stochastic Biochemical Systems p. 151
11:30 – 12:00	<i>Nicolas Nagel</i> Precise asymptotics and exact expressions for QMC-errors of Fibonacci lattices p. 152	<i>Robert Gruhlke</i> A one-shot method for Bayesian optimal experimental design p. 152	<i>Stjepan Salatović</i> Multilevel Gaussian Processes with Applications to Inverse Problems p. 153	<i>Maksim Chupin</i> Tensor Train Decomposition for Optimal Importance Sampling in Stochastic Reaction Networks p. 153
12:00 – 12:30	<i>Marcin Wnuk</i> Regularizing the randomized QMC quadratures via the Median of Means. p. 154	<i>André-Alexander Zepernick</i> From Flat to Curved: UQ for PDEs on Random Surfaces using QMC p. 155	<i>M. Croci</i> Level-set approximation of noisy functions p. 155	
12:30 – 14:00	Lunch Break (JCMB Magnet Café, 3217, 3211)			
14:00 –	Free Afternoon			

Friday June 12th

09:00 – 10:00	Swann Main Lecture Theatre Plenary Talk (PT07) <i>Marylou Gabrié</i> “Assisting sampling of physical systems and Bayesian Inference with generative models” p. 34 Chair: <i>Jonas Latz</i>		
10:00 – 10:30	Coffee Break (JCMB Magnet Café)		
10:30 – 12:30	JCMB 5327 Technical Session (CT11) Bayesian methods Chair: <i>Nathan Kirk</i>	JCMB 5328 Technical Session (CT12) Point sets Chair: <i>Christian Weiß</i>	JCMB 6206 Technical Session (CT09) Approximation Chair: <i>Aretha Teckentrup</i>
10:30 – 11:00	<i>Nathan Kirk</i> A Bayesian Approach to Low Discrepancy Subset Selection p. 156	<i>Christian Weiß</i> Uniform Distribution in the p-adic Integers and Applications p. 156	<i>Carsten Steiber</i> Asymptotic error bounds for numerical integration of infinite-variate functions in tensor product RKHS p. 157
11:00 – 11:30	<i>Andi Q. Wang</i> Markov category Monte Carlo: a categorical account of Metropolis–Hastings p. 157	<i>Christiane Lemieux</i> On choosing parameters for Kronecker sequences p. 158	<i>Pascal Schröter</i> Learning Anisotropy Parameters to Improve ANOVA Approximations p. 159
11:30 – 12:00	<i>Maarten Volkaerts</i> MCMC for Bayesian inference of the non-conducting region in intra-atrial reentrant tachycardia p. 159	<i>Zonghao (Hudson) Chen</i> Stationary MMD Points p. 160	<i>Edoardo Bandoni</i> Optimal Sampling for Kernel Quadrature on Unbounded Domains p. 160
12:00 – 12:30		<i>Vincent Liang</i> A trapezoidal quadrature scheme for fractional Brownian motion p. 161	<i>Lorenzo Calzolari</i> Space-filling designs in the unit ball of a Reproducing Kernel Hilbert Space p. 161
12:30 – 14:00	Lunch Break (JCMB Magnet Café, 3217, 3211)		
14:00 –	Free Afternoon		

Tutorials

Monday June 8th – Morning, 09:15 – 10:45, Swann Main Lecture Theatre

A Primer on Importance Sampling and Particle Filters

Chair: Aretha Teckentrup

Víctor Elvira

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This tutorial provides an introduction to importance sampling and particle filters, two fundamental Monte Carlo methodologies for Bayesian inference and dynamical systems. We first review the principles of importance sampling, including proposal design, weighting mechanisms, variance considerations, and adaptive strategies. We then introduce particle filtering methods for sequential inference in state-space models, covering propagation, weighting, resampling, and practical implementation aspects. The tutorial emphasizes intuition, methodological foundations, and practical challenges arising in high-dimensional, nonlinear, and non-Gaussian problems. Connections with modern applications in computational statistics, machine learning, and climate science will also be discussed.

Monday June 8th – Morning, 11:15 – 12:45, Swann Main Lecture Theatre

Introduction to Quasi-Monte Carlo

Chair: Aretha Teckentrup

Christiane Lemieux

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We provide an overview of key aspects of quasi-Monte Carlo methods, and why this alternative to Monte Carlo methods often provides superior performance for numerical integration and other computational tasks. We review different constructions, randomizations, error and variance bounds, and also discuss more practical aspects and some recent developments.

Plenary Talks

Monday June 8th – Afternoon/1, 14:00 – 15:00, Swann Main Lecture Theatre

Random fields and stochastic partial differential equations on hypersurfaces

Chair: Sara Wade

Annika Lang

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Looking around us, many surfaces including the Earth are no plain Euclidean domains but special cases of Riemannian manifolds. Uncertain physical phenomena on these surfaces can for example be described by random fields and stochastic partial differential equations. In this talk, I will introduce these stochastic quantities on hypersurfaces. Furthermore, I will discuss their efficient simulation and show how the obtained samples can be used to generate random shapes and time-evolving stochastic manifolds.

Tuesday June 9th – Morning/1, 09:00 – 10:00, Swann Main Lecture Theatre

Micromodal posteriors: existence, escape and model-misspecification

Chair: Konstantinos Zygalakis

Gareth Roberts

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Coauthor(s): Sanket Agrawal and Sebastiano Grazi

In Bayesian Statistics, the use of heavy-tailed error models is often attractive for robustness and differential privacy. However there are consequences for such a choice. The effect of outliers on posterior models of this type is to create “micromodes” in the tail of the posterior distribution. Therefore while Bernstein von-Mises Theorem still holds, the posterior will (with high probability) be multi-modal, albeit with the minor modes having mass which recedes to 0 rapidly as the data set size grows. While independent draws from such a posterior will almost certainly not see these minor modes, MCMC algorithms designed to explore the posterior could potentially be affected by them. Since PDMP methods have some claims to escape modes more effectively than many other MCMC methods, we shall explore

the effect of micromodes on the transient phase of the Zig-Zag sampler on simple heavy-tailed regression models. We introduce the notion of an “essential” micromode which has

the property that the sampler takes longer to escape the mode than to return to stationarity if that model were absent. When using t errors, when the data is no heavier than the model used, we find that essential micromodes cannot exist. However in the misspecified case where the data is heavier than the model being used, essential micromodes do exist with high probability, potentially leading to catastrophic MCMC performance. This presentation will cover work largely contained in [1].

[1] Agrawal S, Grazi S and Roberts GO. On micromodes in Bayesian posterior distributions and their implications for MCMC. arXiv preprint arXiv:2602.06931.

Tuesday June 9th – Afternoon/1, 14:00 – 15:00, Swann Main Lecture Theatre

Empirical PAC-Bayes bounds for Markov chains

Chair: Chris. J. Oates

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Coauthor(s): Vahe Karagulyan

Among all the theoretical approaches developed to control the generalization error of classification and regression algorithms in machine learning, PAC-Bayes bounds have a special connection with Bayesian inference. In particular, they provide theoretical ground for various kinds of generalized posteriors, including fractional posteriors and variational approximations. Unfortunately, most of the generalization theory in machine learning (PAC-Bayes or not!) was developed for i.i.d. observations only. While there are a few exceptions, the few PAC and PAC-Bayes bounds known for time series are not distribution-free: they require the knowledge of some mixing coefficients, which is a serious limitation to their application.

I will begin the talk by a quick introduction to PAC-Bayes bounds. I will especially discuss the connections to variational inference. In a second time, I will discuss extensions of this approach to time series. I will introduce a new PAC-Bayes bound for Markov chains. This bound depends on a quantity called the pseudo-spectral gap. The main novelty is that, at least in some favorable situations, we can provide an empirical bound on the pseudo-spectral gap. This leads to fully empirical PAC-Bayes bound for Markov chains. I will finally discuss possible extensions beyond the Markov case.

[1] P. Alquier. User-friendly introduction to PAC-Bayes bounds. *Foundations and Trends in Machine Learning*, 2024, vol. 17, no. 2, pp. 174-303.

[2] V. Karagulyan & P. Alquier. Empirical PAC-Bayes bounds for Markov chains. *Proceedings of the 29th International Conference on Artificial Intelligence and Statistics (AISTATS)*, *Proceedings of Machine Learning Research*, 2026, vol. 300 (to appear).

Wednesday June 10th – 1, 09:05 – 10:00, Swann Main Lecture Theatre

Where Quasi-Monte Carlo Theory and Practice Meet

Chair: Abdul-Lateef Haji-Ali

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Quasi-Monte Carlo (QMC) methods are underpinned by deep mathematical theory and have demonstrated high-impact computational performance. A wide range of low-discrepancy sequences and QMC algorithms have been developed and implemented in modern software libraries.

Despite this progress, key challenges remain: selecting effective sequences for real problems, formulating computations to fully exploit QMC structure, and developing reliable, data-driven error assessment.

This talk examines these challenges through the lens of both theory and practice, offering perspectives on how the two can be more tightly integrated and where future advances may emerge.

Thursday June 11th – Morning/1, 09:00 – 10:00, Swann Main Lecture Theatre

How to recover a function: optimal methods and theoretical guarantees

Chair: Aretha Teckentrup

Kateryna Pozharska

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Coauthor(s): Tino Ullrich and Moritz Moeller

We study reconstruction algorithms (decoders) for unknown high-dimensional relations.

The talk presents an overview on function recovery methods based on different types of data: point evaluations (samples) versus general linear measurements, such as coefficients with respect to a given basis or redundant system. A central theme is the role of the decoder itself, in particular the distinction between linear and non-linear reconstruction methods.

As a typical linear reconstruction approach, we consider a (weighted) least squares method for sampling recovery. In contrast, we discuss non-linear decoders arising from compressive sensing and sparse recovery, including square-root Lasso (rLasso), Orthogonal Matching Pursuit (OMP), and Compressive Sampling Matching Pursuit (CoSaMP). For these methods, we present theoretical guarantees, compare their performance, and analyze their optimality in various model settings.

Our results show that, in certain situations, function values can be as informative as general linear measurements and, when combined with non-linear decoders, can even outperform purely linear reconstruction algorithms. We further discuss implications for related problems, including high-dimensional quadrature and frame discretization.

Thursday June 11th – Afternoon/1, 14:00 – 15:00, Swann Main Lecture Theatre

Stochastic Simulation Perspectives on AI: Global Dynamics of SGD and Average-Reward Reinforcement Learning

Chair: Neil Chada

Chang-Han Rhee

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Coauthor(s): Mihail Bazhba, Jose Blanchet, Bohan Chen, Jeffrey Wang, Xingyu Wang, Bert Zwart

Modern artificial intelligence (AI) is built on fundamentally stochastic components, and mathematical tools from stochastic simulation offer powerful theoretical lenses and algorithmic foundations for understanding and improving AI systems. This talk explores two problems at the intersection of simulation methodologies and machine learning.

In the first part, I will discuss the global dynamics of stochastic gradient descent (SGD) and its variants. The empirical success of deep learning is often attributed in part to the remarkable ability of SGD and its variants to avoid sharp local minima in the loss landscape, since sharp minima are believed to lead to poor generalization. To unravel this mystery and potentially further enhance this capability further, it is imperative to go beyond the traditional local convergence analysis and obtain a comprehensive understanding of SGDs' global dynamics in complex nonconvex loss landscapes. Building on a framework that combines heavy-tailed large deviations with local stability analysis, we characterize the global dynamics of SGD. We also reveal a fascinating phenomenon: by injecting and then truncating heavy-tailed noise during the training, SGD can almost completely avoid sharp minima and often achieve better test-set generalization.

In the second part, I will discuss gradient estimation for average-reward reinforcement learning. In the sequential optimization setting, we examine reinforcement learning (RL) with a long-run average-reward objective. While recent efforts have successfully adapted trust-region methods to the average-reward setting, these algorithms remain highly vulnerable to instability in unbounded state spaces—such as queueing networks—due to slow mixing times and inaccurate initial value-function approximations. To overcome this, we propose a multi-scale, average-reward, trust-region-based RL algorithm. By leveraging an L-skeleton Markov Decision Process framework, our approach reduces the effective mixing time and mitigates the cold-start bias of the critic. This yields an unbiased and efficient gradient estimator for the steady-state mean and guarantees stable policy improvement without relying on artificial discounting or heuristic interventions.

Friday June 12th, 09:00 – 10:00, Swann Main Lecture Theatre

Assisting sampling of physical systems and Bayesian Inference with generative models

Chair: Jonas Latz

Marylou Gabrié

École Normale Supérieure

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Deep generative models parametrize very flexible families of distributions able to fit complicated datasets of images or text. These models provide independent samples from complex high-distributions at negligible costs. On the other hand, sampling exactly a target distribution, such the Boltzmann distribution of a physical system or a Bayesian posterior, is typically challenging: either because of dimensionality, multi-modality, ill-conditioning or a combination of the previous. In this talk, I will discuss opportunities and challenges in enhancing traditional inference and sampling algorithms with learning.

Special Sessions

Monday June 8th – Afternoon/1, 15:30 – 17:30, JCMB Lecture Theatre A

Stochastic computation and complexity, Part 1

Organizers:

Larisa Yaroslavtseva

University of Graz

larisa.yaroslavtseva@uni-graz.at

Session Description:

The session is devoted to algorithms and complexity for quadrature of SDEs and SPDEs, in particular under nonstandard assumptions, approximation of stochastic processes, -high and infinite dimensional integration and approximation, including aspects of lower bounds and connections to functional analysis and stochastic analysis.

Andreas Neuenkirch, “Strong convergence rates for a Lie-Trotter splitting scheme for the CIR process” p. 59

Christopher Rauhögger, “On Tamed Euler Schemes for Multidimensional SDEs with a Discontinuous Drift Coefficient” p. 61

Sotirios Sabanis, “When Potentials Get Rough: Langevin & Diffusion Sampling in Semi-Convex Settings” p. 64

Konstantinos Dareiotis, “Itô perspective on variance renormalisation” p. 66

Monday June 8th – Afternoon/1, 15:30 – 17:30, JCMB Lecture Theatre B

Rare event simulation for quantifying climate uncertainties: theory and practice

Organizers:

Fédéric Cérou

Inria and Université de Rennes

Frederic.Cerou@inria.fr

Patrick Héas

Inria and Université de Rennes

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Session Description:

The aim of the session is to bring together specialists of climate and rare event simulations, and show how recent theoretical developments can improve current state of the art uncertainty quantification.

The session will be divided in four talks. The first two talks, by J. Wouters and F. Ragone, will be focused on critical applications of Sequential Monte-Carlo rare event simulation for climate sciences, with a focus respectively on heatwaves and precipitation, and then on sea ice and weakening and collapse of the Atlantic Meridional Overturning Circulation.

This will be followed by M. Rousset with a theoretical introduction about theoretical tools used to minimise the asymptotic variance of the SMC estimator by optimising the importance functions within a parametric family using a stochastic gradient. P. Heas will then develop this approach, and show the first numerical results on simple models, yet aimed at mimicking the behaviour of those used in climate sciences.

<i>Jeroen Wouters</i> , “Efficient Sampling of Extreme Heatwaves and Rainfall in an Intermediate-Complexity Climate Model”	p. 60
<i>Francesco Ragone</i> , “Rare event sampling of Arctic sea ice reduction and collapse of the Atlantic Meridional Overturning Circulation”	p. 62
<i>Mathias Rousset</i> , “Estimation of the Variance Landscape in Multinomial Sequential Monte Carlo Sampling”	p. 64
<i>Patrick Héas</i> , “Numerical study of a variance optimisation algorithm in sequential Monte-Carlo”	p. 66

Monday June 8th – Afternoon/1, 15:30 – 17:30, JCMB Lecture Theatre C

Advances in slice sampling and related methodologies

Organizers:

Mareike Hasenpflug
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Philip Schär
University of Potsdam
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Session Description:

Slice samplers are a family of Markov chain Monte Carlo (MCMC) methods based on the idea of using a slicing auxiliary random variable that enables exploring the target distribution by means of the superlevel sets of its density. Due to this construction, slice samplers are naturally gradient-free. Moreover, compared to other MCMC methods, slice samplers are usually less sensitive to the tuning of hyperparameters and to certain properties of the target distribution, which may be e.g. the dimension of its domain, multimodality, anisotropy or heaviness of tails. Recent years have seen progress in theoretically grasping this robustness of slice samplers, as well as methodological innovations that extend their scope of application. In this session we explore some of these developments, such as the methodological incorporation of Riemannian geometry and the use of approximations of the target distribution, as well as the investigation of spectral properties.

<i>Kevin Bitterlich</i> , “Slice Sampling using Approximations”	p. 60
<i>Cameron Bell</i> , “Advances in Stereographic Slice Sampling”	p. 62

Bernardo Williams, “Geodesic Slice Sampler for Multimodal Distributions with Strong Curvature” p. 65

Philip Schär, “Spectral gap of uniform and geodesic slice sampling on the sphere” p. 67

Monday June 8th – Afternoon/1, 15:30 – 17:30, JCMB 5326

Markov operators for data generation and inference based on denoising diffusions

Organizers:

Marina Riabiz

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Session Description:

Diffusion-based models have become a central paradigm in generative AI, leveraging the observation that corrupting data with noise is straightforward, while learning to reverse this process enables data generation from noise [1-3]. Reversing the diffusion dynamics requires access to the score function of the time-marginal distributions of the perturbed data. Since this quantity is generally unavailable in closed form, it is commonly approximated using neural networks trained to optimize score-matching objectives on samples from the forward noising process.

In this session, we review recent advances that emphasize the advantages of adopting Markov noise processes. Using the theory of Markov operators, one can:

1. Characterize the temporal evolution of expectations of test functions using only expectations with respect to the data distribution. This leads to score estimators derived from the eigendecomposition of Markov operators, potentially eliminating the need to train neural networks to approximate the score [4];
2. Provide a natural framework for defining gradual diffusion processes on non-Euclidean data. In this setting, training neural networks to learn the underlying Markov operators, rather than the score function, enables reversal of the noising process while preserving the intrinsic topological structure of the data [5];

Beyond generative modeling, a growing body of work has adapted diffusion-based techniques to problems in statistical computation, including sampling from and inference for unnormalized distributions, the primary distinction between the two frameworks being the availability of training data [6-7]. In this session, we also showcase forthcoming work that investigates variance reduction for Monte Carlo estimators by exploiting the representation of expectation dynamics enabled by the theory of Markov operators [8].

- [1] Y. Song and S. Ermon. Generative Modeling by Estimating Gradients of the Data Distribution. In Proceedings of the 33rd Conference on Neural Information Processing Systems, 2019.

- [2] J. Ho, A. Jain, and P. Abbeel. Denoising diffusion probabilistic models. In Proceedings of the 34th Conference on Neural Information Processing Systems, pages 6840–6851, 2020.
- [3] Y. Song, J. Sohl-Dickstein, D. P. Kingma, A. Kumar, S. Ermon, and B. Poole. Score-Based Generative Modeling through Stochastic Differential Equations. In Proceedings of the 8th International Conference on Learning Representations, 2020.
- [4] Shen, Z., Wang, H., Riabiz, M. and Oates, C.J., 2024. Operator-informed score matching for Markov diffusion models. arXiv preprint arXiv:2406.09084.
- [5] Stephenson, A., Gallagher, I. and Nemeth, C., 2026. Generator-based Graph Generation via Heat Diffusion. arXiv preprint arXiv:2602.03612.
- [6] Vargas, F., Grathwohl, W. and Doucet, A., 2023. Denoising diffusion samplers. arXiv preprint arXiv:2302.13834.
- [7] Young, J.M., Cordero-Encinar, P., Reich, S., Duncan, A. and Akyildiz, O.D., 2026. Diffusion Path Samplers via Sequential Monte Carlo. arXiv preprint arXiv:2601.21951.
- [8] Wang, H., Shen, Z., Riabiz, M. and Oates, C.J., 2024. Markov operator-informed control variates for denoising diffusion samplers. Forthcoming.

<i>Zheyang Shen</i> , “Structurally-informed diffusion modeling”	p. 61
<i>Huihui Wang</i> , “Operator-informed control variates for denoising diffusion samplers”	p. 63
<i>Chris Nemeth</i> , “Generator-based Graph Generation via Heat Diffusion”	p. 65

Monday June 8th – Afternoon/2, 15:30 – 17:30, JCMB 5327

Gradient Flow for Sampling

Organizers:

Sifan Liu

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Jun Yang

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Session Description:

Gradient flow formulations provide a unifying framework for modern sampling algorithms by viewing probability measures as evolving along the gradient flows of suitable energy functionals, such as entropy or Kullback–Leibler divergence. This perspective connects Markov chain Monte Carlo, Langevin dynamics, interacting particle systems, and optimal transport, offering new insights into algorithm design and analysis.

This invited session highlights recent advances in gradient-flow-based sampling, including theoretical guarantees, convergence and complexity analysis, and scalable particle-based methods for high-dimensional and non-convex targets. Emphasis will be placed on

both rigorous foundations and practical algorithms, with applications to Bayesian inference, statistical physics, and machine learning. The session aims to foster interaction between the Monte Carlo, optimal transport, and applied analysis communities and to identify emerging directions for gradient-flow-inspired sampling methods.

- Louis Sharrock*, “Tuning-Free Sampling via Optimization on the Space of Probability Measures” p. 68
- Francesca R. Crucinio*, “A gradient flow interpretation of sequential Monte Carlo” p. 69
- Rocco Caprio*, “Maximum marginal likelihood, EM, Gradient flows and a log-Sobolev inequality” p. 71
- Mengxin Xi*, “De-biased Simulation of the Mean Field Langevin Dynamics” p. 72

Tuesday June 9th – Morning/1, 10:30 – 12:30, JCMB Lecture Theatre A

Stochastic computation and complexity, Part 2

Organizers:

Larisa Yaroslavtseva
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Session Description:

The session is devoted to algorithms and complexity for quadrature of SDEs and SPDEs, in particular under nonstandard assumptions, approximation of stochastic processes, -high and infinite dimensional integration and approximation, including aspects of lower bounds and connections to functional analysis and stochastic analysis.

- Klaus Ritter*, “Uniform approximation of infinite-variate functions from weighted Hilbert spaces” p. 73
- Toni Karvonen*, “Piecewise linear interpolation and the trapezoidal rule via kernels” p. 75
- Stefan Heinrich*, “On the quantum complexity of parametric integration in Sobolev spaces” p. 78

Tuesday June 9th – Morning/1, 10:30 – 12:30, JCMB Lecture Theatre B

Frontiers in QMC methods, Part 1

Organizers:

Josef Dick
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Takashi Goda
The University of Tokyo
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Kosuke Suzuki
Yamagata University
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Session Description:

This special session highlights recent progress at the interface of numerical integration, QMC approximation, discrepancy theory and information-based complexity, with a particular focus on how quantitative uniformity of point sets governs the performance of algorithms for high-dimensional numerical integration and function approximation. We will discuss modern constructions and analyses—spanning lattice and polynomial lattice methods, digital nets, and related randomized or hybrid variants—that yield dimension-robust error guarantees in weighted and smooth function spaces. By connecting geometric uniformity, complexity theory, and concrete algorithm design, the session aims to foster cross-fertilization between discrepancy, tractability, and practical numerical methods, and to outline emerging directions and open problems for the MC/QMC community.

Friedrich Pillichshammer, “Curse of dimensionality vs. tractability for discrepancy – a survey” p. 74

Zhijian He, “Uncertainty quantification using importance-sampled quasi-Monte Carlo with dimension-independent convergence rates” p. 76

Mou Cai, “The L_p approximation using multiple lattice based algorithm” p. 78

Tuesday June 9th – Morning/1, 10:30 – 12:30, JCMB Lecture Theatre C

Sampling and Machine Learning**Organizers:**

Nathan Kirk

University of St Andrews

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T. Konstantin Rusch

Max Planck Institute for Intelligent Systems & ELLIS Institute Tübingen

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Session Description:

This special session presents recent developments in sampling, approximation, and learning-based numerical methods intersecting quasi-Monte Carlo, stochastic simulation, and machine learning. Topics include the generation of low-discrepancy point sets using graph neural networks in Message-Passing Monte Carlo (MPMC) [1], the construction of low-discrepancy sequences in Neural Low-Discrepancy Sequences (NeuroLDS) [2], reinforcement learning approaches for adaptive proposal design in Markov chain Monte Carlo [3], and the use of antithetic and randomized quasi-Monte Carlo methods for variance reduction in diffusion models [4]. Complementing these developments, the session also includes recent work on Fourier Neural Operators implemented on rank-1 lattices, where quasi-Monte Carlo point sets are used to improve approximation and generalization performance. Collectively, the session highlights current research on the development and use of *learned* constructions for problems arising in numerical integration, uncertainty quantification, Bayesian computation, operator learning, and generative modeling.

- [1] T. K. Rusch, N. Kirk, M. Bronstein, C. Lemieux, D. Rus, *Message-Passing Monte Carlo: Generating low-discrepancy point sets with graph neural networks*, PNAS 121(40), e2409913121 (2024)

- [2] M. Etienne Van Huffel, N. Kirk, M. Chahine, D. Rus, T. K. Rusch, *Neural Low-Discrepancy Sequences*, arXiv Preprint 2510.03745 (2025)
- [3] C. Wang, W. Chen, H. Kanagawa, C. Oates, *Reinforcement learning for adaptive MCMC*, arXiv Preprint 2405.13574 (2024)
- [4] J. Jia, S. Liu, B. Song, W. Yuan, L. Shen, G. Wang, *Antithetic Noise in Diffusion Models*, arXiv Preprint 2506.06185 (2025)

<i>T. Konstantin Rusch</i> , “Neural Quasi-Monte Carlo”	p. 74
<i>Marcelo Pereyra</i> , “Almost nearly perfect Bayesian imaging with physics-informed deep generative models”	p. 76
<i>Sifan Liu</i> , “Quasi-random Sampling in Diffusion Models”	p. 79
<i>Björn Sprungk</i> , “Flow-based Slice Sampling”	p. 80

Tuesday June 9th – Morning/1, 10:30 – 12:30, JCMB 5326

Sampling and approximation for structured stochastic models in scientific computing, Part 1

Organizers:

Conor Osborne
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Session Description:

Sampling and approximation problems for stochastic models are central to uncertainty quantification, inverse problems, and scientific computing. In practice, the efficiency of Monte Carlo methods often depends not only on the sampling algorithm itself, but also on how the underlying stochastic model is represented and approximated. This mini-symposium focuses on structure-exploiting approaches to sampling and approximation for structured stochastic models. Topics include multilevel and multiresolution representations, intrinsic and geometric approximation, operator and covariance structure, and the influence of energy landscapes and model dynamics on sampling behaviour, with an emphasis on how explicit representation choices can be used to improve computational efficiency.

- [1] Niederreiter, Harald (1992). *Random number generation and quasi-Monte Carlo methods*. Society for Industrial and Applied Mathematics (SIAM).
- [2] L’Ecuyer, Pierre, & Christiane Lemieux. (2002). Recent advances in randomized quasi-Monte Carlo methods. *Modeling uncertainty: An examination of stochastic theory, methods, and applications*, 419-474.

<i>Rui-Yang Zhang</i> , “A Dynamic Perspective on Gaussian Processes and the Vanilla-SPDE Exchange”	p. 75
<i>Duc-Lam Duong</i> , “Accelerating posterior sampling in Bayesian inverse problems with score-based diffusion models”	p. 77

Josef Martínek, “Sequential Monte Carlo for Bayesian Inference Using Randomized Likelihoods” p. 79

Tuesday June 9th – Morning/2, 10:30 – 12:30, JCMB 5327

Optimal Experimental Design using Monte Carlo Methods

Organizers:

Jana de Wiljes

Technische Universität Ilmenau

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Philipp Wacker

University of Canterbury

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Session Description:

Optimal Experimental Design for Bayesian Inference is about finding the most suitable experimental setup such that some quantity of interest (usually the information gain) is expected to be maximised for future data yet to be collected under this experimental regime. In this session we will bring together experts working on OED, with a focus on Monte Carlo methods and related fields.

Karina Koval, “On transport approaches to Bayesian optimal experimental design” p. 80

Tim Waite, “Sequential Bayesian design via Laplace policies” p. 82

Jonas Latz, “Sparse Techniques for Regression in Deep Gaussian Processes” p. 84

Tuesday June 9th – Morning/2, 10:30 – 12:30, JCMB 5328

Advances in Monte Carlo methods for rare-event simulation, Part 1

Organizers:

Shyam Mohan Subbiah Pillai

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Nadhir Ben Rached

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Raúl Tempone

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Session Description:

Rare events, though characterized by extremely small probabilities, play a decisive role in a wide range of applications including quantitative finance, wireless communication systems, reliability engineering, and computational biology. Accurately estimating such probabilities poses significant computational challenges, as naive Monte Carlo methods

become prohibitively expensive in the small-probability regime. This mini-symposium focuses on modern variance reduction methodologies designed specifically for rare-event simulation. Emphasis will be placed on advanced techniques such as importance sampling, splitting methods, multilevel strategies, and control variates, particularly in high-dimensional and stochastic dynamical systems. The session aims to highlight both recent theoretical developments and algorithmic innovations in this exciting field.

<i>Nadhir Ben Rached</i> , “Tracking rare events within the ensemble Kalman filtering”	p. 81
<i>Víctor Elvira</i> , “Rare event estimation for multimodal and high-dimensional problems via subset adaptive importance sampling”	p. 82
<i>Carsten Hartmann</i> , “Importance sampling of unbounded random stopping times”	p. 84
<i>Lorenz Richter</i> , “Rare event simulation via stochastic optimal control: new perspectives from diffusion-based sampling”	p. 86

Tuesday June 9th – Afternoon/1, 15:30 – 17:30, JCMB Lecture Theatre A

Stochastic computation and complexity, Part 3

Organizers:

Thomas Müller-Gronbach

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Session Description:

The session is devoted to algorithms and complexity for quadrature of SDEs and SPDEs, in particular under nonstandard assumptions, approximation of stochastic processes, -high and infinite dimensional integration and approximation, including aspects of lower bounds and connections to functional analysis and stochastic analysis.

Iosif Lytras, “Contractive kinetic Langevin samplers beyond global Lipschitz continuity” p. 87

Máté Gerencsér, “Overcoming the temporal and spatial order barriers in approximating space-time white noise-driven SPDEs” p. 89

Laurent Mertz, “A Control Variate Method Driven by Diffusion Approximation” p. 91

Chengcheng Ling, “Weak approximation of kinetic SDEs: closing the criticality gap” p. 93

Tuesday June 9th – Afternoon/1, 15:30 – 17:30, JCMB Lecture Theatre B

Mean Fields, Flows and Sampling

Organizers:

Chris. J. Oates

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Session Description:

Several emerging applications, including mean field games, training of infinite-width neural networks, and post-Bayesian inference, require minimising an objective functional

defined on a space of probability distributions. Accordingly, this session focuses on the interface between sampling and optimisation, with particular emphasis on nonlinear objective functionals for which techniques such as mean field Langevin dynamics are useful.

Nikolas Nüsken, “From optimisation to sampling: beyond gradient flows” p. 88

Mateusz B. Majka, “Non-convex entropic mean-field optimization via Best Response flow” p. 90

Gonçalo dos Reis, “Data-driven approximation of transfer operators for mean-field stochastic differential equations” p. 92

Chris. J. Oates, “A Computable Measure of Suboptimality for Entropy-Regularised Variational Objectives” p. 94

Tuesday June 9th – Afternoon/1, 15:30 – 17:30, JCMB Lecture Theatre C

Sampling and approximation for structured stochastic models in scientific computing, Part 2

Organizers:

Conor Osborne

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Session Description:

Sampling and approximation problems for stochastic models are central to uncertainty quantification, inverse problems, and scientific computing. In practice, the efficiency of Monte Carlo methods often depends not only on the sampling algorithm itself, but also on how the underlying stochastic model is represented and approximated. This mini-symposium focuses on structure-exploiting approaches to sampling and approximation for structured stochastic models. Topics include multilevel and multiresolution representations, intrinsic and geometric approximation, operator and covariance structure, and the influence of energy landscapes and model dynamics on sampling behaviour, with an emphasis on how explicit representation choices can be used to improve computational efficiency.

[1] Niederreiter, Harald (1992). *Random number generation and quasi-Monte Carlo methods*. Society for Industrial and Applied Mathematics (SIAM).

[2] L’Ecuyer, Pierre, & Christiane Lemieux. (2002). Recent advances in randomized quasi-Monte Carlo methods. *Modeling uncertainty: An examination of stochastic theory, methods, and applications*, 419-474.

Jürgen Dölz, “Data-intrinsic approximation in metric spaces” p. 88

Maia Tienstra, “Free Energy Barriers in Bayesian Logistic Regression” p. 90

Conor Osborne, “Efficient sampling of deep Gaussian processes via wavelet sparsity” p. 92

Tuesday June 9th – Afternoon/1, 15:30 – 17:30, JCMB 5326

Interacting and Adaptive Particle Methods for Approximating Complex Distributions

Organizers:

Arne Bouillon

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Session Description:

Sampling and approximating high-dimensional and multimodal probability distributions remains a central challenge in scientific computing, Bayesian inference, and uncertainty quantification. Recent years have seen the rapid development of particle-based and population-based sampling algorithms that combine ideas from stochastic dynamics, importance sampling, optimization, and mixture approximation. This special session focuses on recent advances in adaptive and interacting particle methods that aim to improve sampling efficiency, robustness, and theoretical understanding.

Particular attention is given to methodologies that exploit ensembles of particles to learn and adapt proposal distributions, incorporate interaction mechanisms, and construct flexible approximations of target distributions. By integrating ideas from adaptive importance sampling, interacting particle dynamics, and sequential mixture construction, these approaches seek to more effectively utilize information contained in particle populations and to improve robustness when sampling from complex distributions. The session aims to stimulate discussion on theoretical properties, algorithmic design, and empirical performance of modern particle-based sampling techniques, with applications across inverse problems, uncertainty quantification, and high-dimensional statistical inference.

Arne Bouillon, “Localized consensus-based sampling” p. 89

Paolo Villani, “Greedy Mixture Approximation: A Unified Algorithmic Framework” p. 91

Ilya Klebanov, “Importance Reweighting of Interacting Particle Samplers” p. 93

Tuesday June 9th – Afternoon/2, 15:30 – 17:30, JCMB 5327

Frontiers in QMC methods, Part 2

Organizers:

Josef Dick

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Takashi Goda

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Kosuke Suzuki

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Session Description:

This special session highlights recent progress at the interface of numerical integration, QMC approximation, discrepancy theory and information-based complexity, with a particular focus on how quantitative uniformity of point sets governs the performance of algorithms for high-dimensional numerical integration and function approximation. We will discuss modern constructions and analyses—spanning lattice and polynomial lattice methods, digital nets, and related randomized or hybrid variants—that yield dimension-robust error guarantees in weighted and smooth function spaces. By connecting geometric uniformity, complexity theory, and concrete algorithm design, the session aims to foster cross-fertilization between discrepancy, tractability, and practical numerical methods, and to outline emerging directions and open problems for the MC/QMC community.

<i>Zexin Pan</i> , “Dimension-independent convergence rates of median randomized nets”	p. 94
<i>Kosuke Suzuki</i> , “Coarse scrambling for Sobol’ and Niederreiter sequences”	p. 96
<i>Ziyang Ye</i> , “A median QMC method for unbounded integrands over \mathbb{R}^s in weighted unanchored Sobolev spaces”	p. 98
<i>Jakob Dilen</i> , “Fourier Neural Operators on Rank-1 Lattices”	p. 99

Tuesday June 9th – Afternoon/2, 15:30 – 17:30, JCMB 5328

Advances in Monte Carlo methods for rare-event simulation, Part 2

Organizers:

Shyam Mohan Subbiah Pillai

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Nadhir Ben Rached

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Raúl Tempone

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Session Description:

Rare events, though characterized by extremely small probabilities, play a decisive role in a wide range of applications including quantitative finance, wireless communication systems, reliability engineering, and computational biology. Accurately estimating such probabilities poses significant computational challenges, as naive Monte Carlo methods become prohibitively expensive in the small-probability regime. This mini-symposium focuses on modern variance reduction methodologies designed specifically for rare-event simulation. Emphasis will be placed on advanced techniques such as importance sampling, splitting methods, multilevel strategies, and control variates, particularly in high-dimensional and stochastic dynamical systems. The session aims to highlight both recent theoretical developments and algorithmic innovations in this exciting field.

<i>Shyam Mohan Subbiah Pillai</i> , “Estimating rare-event probabilities associated with the McKean-Vlasov equation”	p. 95
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Eya Ben Amar, “Hierarchical Importance Sampling for Estimating Occupation Times of SDE Solutions” p. 96

Karthyek Murthy, “Variance Reduction with Importance Sampling for Optimization Under Rare Chance Constraints” p. 98

Wednesday June 10th – 1, 10:30 – 12:30, JCMB Lecture Theatre A

Stochastic computation and complexity, Part 4

Organizers:

Thomas Müller-Gronbach

University of Passau

thomas.mueller-gronbach@uni-passau.de

Session Description:

The session is devoted to algorithms and complexity for quadrature of SDEs and SPDEs, in particular under nonstandard assumptions, approximation of stochastic processes, -high and infinite dimensional integration and approximation, including aspects of lower bounds and connections to functional analysis and stochastic analysis.

Stefano Bruno, “Flatness-Aware Stochastic Gradient and Zeroth-Order Langevin Dynamics” p. 101

Lukasz Stepien, “Exact asymptotic error and optimality of adaptive Milstein scheme for global approximation of SDEs with countably dimensional noise” p. 103

Larisa Yaroslavtseva, “On lower error bounds for strong approximation of SDEs with Hölder continuous drift coefficient” p. 106

Nikolaos Makras, “The Tamed Subgradient Unadjusted Langevin Algorithm beyond Convexity” p. 108

Wednesday June 10th – 1, 10:30 – 12:30, JCMB Lecture Theatre B

Approximation and sampling of concentrated posterior distributions

Organizers:

Daniel Rudolf

Universität Passau

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Björn Sprungk

TU Bergakademie Freiberg

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Session Description:

In Bayesian inference, large sets of observational data or a small observational noise typically lead to strongly concentrated posterior distributions. From a modeling point of view this is a desirable scenario, however from a computational perspective it is also challenging, since most sampling methods suffer from high concentration. Knowledge

about the rate at which the sequence of concentrating posterior distributions converges to its limit is important for the design and guarantees of cheap proxies of the posterior that mimic the same anisotropic concentration behavior such as the Laplace approximation. In this session we discuss recent advances on posterior concentration and convergence of common approximation such as the Laplace Approximation in high dimensions, as well as corresponding implications for efficient sampling based on these approximations.

<i>Maxime Egéa</i> , “A multimodal Laplace approximation”	p. 101
<i>Hanyue Gu</i> , “Multimodal Laplace-based sampling”	p. 104
<i>Anya Katsevich</i> , “High-dimensional Laplace asymptotics up to the concentration threshold”	p. 107
<i>Dana Wrischnig</i> , “Wasserstein Stability of Bayesian Posteriors in the Concentrated Posterior Regime”	p. 109

Wednesday June 10th – 1, 10:30 – 12:30, JCMB Lecture Theatre C

Gradient Flows and Continuous-time Markov Processes in Data Science and Beyond

Organizers:

Ö. Deniz Akyildiz

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Jonas Latz

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Philipp Wacker

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Session Description:

Continuous-time dynamics have received considerable interest in statistics and machine learning in recent years. They usually arise either as statistical models that shall explain continuously or discretely observed data or as continuity limits of algorithms and discrete models. When used as statistical models, challenges are in effective filtering and control, efficient discretisation, and non-parametric statistical guarantees. When used to describe algorithms, e.g., gradient flows as continuity limits of gradient descent on spaces of probability measures, challenges arise in the associated functional/PDE/stochastic analysis, efficient discretisation, and application to machine learning problems. This minisymposium will highlight current work in this area and seek intersections between the fields.

Paula Cordero Encinar, “Diffusion Annealed Langevin Monte Carlo for Generative Modelling and Sampling” p. 102

Philipp Wacker, “An optimal experimental design approach to sensor placement in continuous stochastic filtering” p. 104

Lisa Hickl, “On the Algorithmic and Theoretical Path Towards Optimal Personalised Treatment” p. 107

Joël Tatang Demano, “Piecewise Deterministic Sampling for Constrained Distributions”
p. 109

Wednesday June 10th – 1, 10:30 – 12:30, JCMB 5326

Recent advances in hierarchical methods for uncertainty quantification, Part 1

Organizers:

Arved Bartuska

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Yang Liu

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Session Description:

Quantifying uncertainties in models and applications typically involves numerical estimations of high-dimensional integrals. Monte Carlo (MC) methods provide a sample-based estimate that does not suffer from the curse of dimensionality. Quasi-MC (QMC) methods provide an approximation that converges faster under certain regularity conditions, typically at the expense of a dimension-dependent multiplicative term in the error. Hierarchical methods provide improvements in computational efficiency by harnessing trade-offs between different levels of accuracy of integrand approximations, making highly accurate estimates feasible. This session explores recent advances in hierarchical MC and QMC methods and their applications.

Chiheb Ben Hammouda, “Single- and Multi-Level Fourier-RQMC Methods for Multivariate Shortfall Risk”
p. 102

Louise Kluge, “Hierarchical Delayed Acceptance using Gaussian Process Surrogates”
p. 105

Leon Wilkosz, “Stochastic Optimal Control for a System of Delay Equations arising from Heat and Humidity Control”
p. 108

Riccardo Saporiti, “Multilevel Markov chain Monte Carlo for a class of partially observed diffusions with noiseless observations”
p. 110

Wednesday June 10th – 2, 10:30 – 12:30, JCMB 5327

Sample Points: Quality Measures, Constructions, and Applications

Organizers:

Michael Gnewuch

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Peter Kritzer

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Session Description:

Sampling in high-dimensions plays an important role in numerical integration, simulation, optimization, function approximation, and other areas of mathematics. Depending on the application, there are different techniques for the generation of such point sets and sequences which are often based on methods from probability theory as well as number theory. In applications in the natural sciences and in computer science there are usually different requirements that “good point sets” should satisfy. Quality criteria of common interest comprise, e.g., a low error, low discrepancy, or small energy norms. In this special session we will bring together distinguished researchers working on the solution of high-dimensional computational problems and/or discrepancy theory to discuss different quality criteria for selecting sample points, algorithms based on these, their theoretical properties, and their performance in applications.

<i>Dmitriy Bilyk</i> , “Energies with Tensor Product Structure, Fibonacci Lattices, and One-Distance Sets on the Torus”	p. 111
<i>Yoshihito Kazashi</i> , “Optimality of quasi-Monte Carlo methods and suboptimality of the sparse-grid Gauss–Hermite rule”	p. 114
<i>Dirk Nuyens</i> , “Multi-fidelity quasi-Monte Carlo”	p. 115
<i>Ian H. Sloan</i> , “Doubling the convergence rate with kernel approximation”	p. 117

Wednesday June 10th – 2, 10:30 – 12:30, JCMB 5328

MLMC for SPDEs

Organizers:

Mike Giles

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Abdul-Lateef Haji-Ali

Heriot-Watt University

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Session Description:

In this session we look at the analysis of Multilevel Monte Carlo methods applied to stochastic PDEs, including different ways of generating appropriately coupled noise samples of various types on multiple grid levels.

<i>Abdul-Lateef Haji-Ali</i> , “Hierarchical Methods for Semilinear Stochastic Partial Differential Equations”	p. 111
<i>Annika Lang</i> , “Sampling the “same” coloured noise on different grid levels”	p. 115
<i>Mike Giles</i> , “Different MLMC treatments of the stochastic heat equation”	p. 116

Thursday June 11th – Morning/1, 10:30 – 12:30, JCMB Lecture Theatre A

Complexity of high-dimensional approximation

Organizers:

Peter Kritzer

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Mathias Sonnleitner

University of Münster and University of Bielefeld

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Session Description:

High-dimensional approximation problems lie between the curse of dimensionality and surprising forms of tractability. This session focuses on recent progress in information-based complexity that clarifies how achievable approximation rates depend on the type of information used - such as function values, randomization, or nonlinear measurements. Emphasis is placed on the interaction between tractability theory and discrepancy, approximation in kernel-based function spaces, including weighted and Gaussian settings, and on identifying conditions under which dimension-robust or nearly dimension-independent complexity bounds can be achieved.

Speakers:

- Peter Kritzer, RICAM, Austrian Academy of Sciences
- Moritz Moeller, University of Technology Chemnitz
- Erich Novak, University of Jena
- Yuya Suzuki, Aalto University

Erich Novak, “Numerical Integration and its Complexity for Functions with Uniformly Bounded Derivatives” p. 118

Yuya Suzuki, “Approximation of differential entropy in Bayesian optimal experimental design” p. 120

Moritz Moeller, “Instance optimal sampling recovery and minimal number of samples” p. 122

Peter Kritzer, “ L_2 -approximation using median lattice algorithms” p. 125

Thursday June 11th – Morning/1, 10:30 – 12:30, JCMB Lecture Theatre B

New developments in quasi-Monte Carlo methods, Part 1

Organizers:

Zexin Pan

Zhejiang University

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Zhijian He

South China University of Technology
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Session Description:

Our session presents seven talks on the latest QMC developments. We will cover theoretical advances, such as improved upper bounds on star discrepancy and new constructions of QMC point sets, alongside practical applications in machine learning, finance engineering and SDE simulations.

- Josef Dick*, “The star discrepancy of a union of randomly digitally shifted Korobov (polynomial) lattice point sets depends polynomially on the dimension” p. 118
- Takashi Goda*, “Space-filling lattice designs for computer experiments” p. 120
- Du Ouyang*, “Quasi-Monte Carlo for SDE Simulation: Error Analysis and Dimensionality Reduction” p. 123
- Jianlong Chen*, “Convergence Analysis for Generative Models with Quasi-Monte Carlo Importance Sampling” p. 125

Thursday June 11th – Morning/1, 10:30 – 12:30, JCMB Lecture Theatre C

Probabilistic couplings for the design and analysis of Monte Carlo methods

Organizers:

Shiva Darshan
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Session Description:

Couplings are a versatile tool in modern probability theory. Among many other applications, they have been fruitfully applied in the last thirty years to prove quantitative upper bounds on the convergence rates of a wide range of Markov Chain Monte Carlo methods. More recently, various authors have used explicit couplings to improve existing MCMC methods and design new methods, for example unbiased MCMC methods [4, 6, 1], online convergence diagnostics [7, 2], and coupling-based control variates [8, 5, 3]. This session aims to advertise the utility of couplings to others parts of the MCMC community and to showcase some recent progress on couplings and their applications to a variety of MCMC methods.

- [1] Y. F. Atchadé and P. E. Jacob. Unbiased Markov Chain Monte Carlo: what, why, and how. *Preprint*, arXiv:2406.06851.
- [2] N. Biswas, P. E. Jacob, and P. Vanetti. Estimating convergence of Markov chains with L-lag couplings. *Advances in Neural Information Processing Systems*, 2019.
- [3] S. Darshan, A. Eberle, and G. Stoltz. Sticky coupling as a control variate for sensitivity analysis. *Preprint*, arXiv:2409.15500.
- [4] P. W. Glynn and C.-H. Rhee. Exact estimation for Markov chain equilibrium expectations. *Journal of Applied Probability*, 2014.

- [5] J. B. Goodman and K. K. Lin. “Coupling control variates for Markov chain Monte Carlo”. In: *Journal of Computational Physics*, 2009.
- [6] P. E. Jacob, J. O’Leary, and Y. F. Atchadé. Unbiased Markov chain Monte Carlo methods with couplings. In: *Journal of the Royal Statistical Society: Series B*, 2020.
- [7] V. E. Johnson. Studying convergence of Markov Chain Monte Carlo algorithms using coupled sample paths. *Journal of the American Statistical Association*, 1996.
- [8] R. M. Neal and R. L. Pinto. Improving Markov chain Monte Carlo estimators by coupling to an approximating chain. *Preprint*, Tech. rep. 0101 Department of Statistics, University of Toronto, 2001.

Adrien Corenflos, “Computing importance weights for Markov chain Monte Carlo via couplings: an application to f-divergence diagnostics” p. 119

Peter A. Whalley, “Scalable Langevin Monte Carlo Methods for Bayesian Inference” p. 121

Tamás P. Papp, “Scaling couplings of Markov chain Monte Carlo algorithms to high dimensions” p. 123

Joonas Karjalainen, “Mixing time of the conditional backward sampling particle filter” p. 126

Thursday June 11th – Morning/1, 10:30 – 12:30, JCMB 5326

Practical aspects of Monte Carlo simulation in applications

Organizers:

Emil Løvbak

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Josef Martínek

Heidelberg University
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Session Description:

This minisymposium explores the development and application of particle-based simulations for solving complex problems in science and engineering governed by (integro-)differential equations. The session covers the full scope of particle-based modeling, from foundational computational infrastructure to specialized numerical implementations and applications including nuclear fusion, radiation therapy or medical imaging. Discussions will focus on enhancing simulation performance, developing robust models for complex systems, and ensuring the reliability of results. By bringing together researchers from diverse disciplines, this symposium aims to address current progress and shared challenges in the field of particle-based simulations.

Sidney Hansen, “Rendering volumes with bitmasks” p. 119

Thijs Steel, “Artificially reduced collisionality Monte Carlo, an approximation method for neutral particles in the plasma edge of a fusion reactor” p. 122

Dániel Hajnal, “Multifidelity Uncertainty Quantification for Photon Radiotherapy” p. 124

Caleb Sbani, “Reversing SPRNG: on Reversible Pseudorandom Number Generators”
p. 126

Thursday June 11th – Morning/2, 10:30 – 12:30, JCMB 5327

Recent Advances in Gibbs Sampling

Organizers:

Andi Q. Wang

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Session Description:

The Gibbs sampler is one of the oldest and most foundational Markov chain Monte Carlo methods, enabling sampling from a complex probability distribution whenever it possesses tractable conditional distributions. It remains extremely popular in practice, and despite being thoroughly well-studied, there have been a number of exciting theoretical breakthroughs in recent years. In this session, we will discuss several significant contributions advancing our understanding of Gibbs samplers, with results covering systematic- and random-scan samplers, and related hybrid data augmentation and slice sampling chains. These advances have been made using a variety of tools and techniques. These include: analysis of nonreversible two-component systematic scan samplers into the setting of vanishing or absent spectral gaps using the framework of weak Poincaré inequalities, presented by Mengxi Gao; work on spectral gap decompositions, providing guarantees even for non-reversible systematic scan samplers, presented by Qian Qin; recent developments in the application of transport maps and isoperimetry to give state-of-the-art convergence guarantees, presented by Giacomo Zanella.

Mengxi Gao, “Weak Poincaré inequalities for Deterministic-scan Metropolis-within-Gibbs samplers” p. 127

Qian Qin, “On spectral decomposition for Markov chains” p. 129

Cecilia Secchi, “Spectral gap of Metropolis-within-Gibbs under log-concavity” p. 130

Thursday June 11th – Afternoon/1, 15:30 – 17:30, JCMB Lecture Theatre A

Stochastic computation and complexity, Part 6

Organizers:

Stefan Heinrich

RPTU, University Kaiserslautern

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Session Description:

The session is devoted to algorithms and complexity for quadrature of SDEs and SPDEs, in particular under nonstandard assumptions, approximation of stochastic processes, high and infinite dimensional integration and approximation, including aspects of lower bounds and connections to functional analysis and stochastic analysis.

<i>Fred J. Hickernell</i> , “Good Lattice and Kronecker Sequences for Arbitrary Sample Size”	p. 133
<i>Daniel Rudolf</i> , “Gibbsian polar slice sampling”	p. 135
<i>Michael Gnewuch</i> , “Optimality of QMC Quadrature Rules on Multiple Scales of Function Spaces”	p. 136
<i>Leszek Plaskota</i> , “Optimal approximation of piecewise smooth functions from information contaminated with random noise”	p. 138

Thursday June 11th – Afternoon/1, 15:30 – 17:30, JCMB Lecture Theatre B

New developments in quasi-Monte Carlo methods, Part 2

Organizers:

Zexin Pan

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Zhijian He

South China University of Technology

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Session Description:

Our session presents seven talks on the latest QMC developments. We will cover theoretical advances, such as improved upper bounds on star discrepancy and new constructions of QMC point sets, alongside practical applications in machine learning, finance engineering and SDE simulations.

Yu Xu, “Nested Multilevel Monte Carlo with Preintegration for Efficient Risk Estimation”
p. 134

Yang Liu, “Quasi-Monte Carlo with a Hankel random digital net”
p. 135

Valerie Ho, “Randomized Quasi-Monte Carlo for Walk on Spheres”
p. 137

Thursday June 11th – Afternoon/1, 15:30 – 17:30, JCMB Lecture Theatre C

Bayesian inference using Monte Carlo and quasi-Monte Carlo methods

Organizers:

Laura Bazahica

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Vesa Kaarnioja

LUT University

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Session Description:

Computational measurement models may involve several unknown or uncertain simulation parameters such as the material properties of a heterogeneous medium or the shape

of the structure itself. In many practical problems, we have measurement data of the outcomes of these measurement models and we wish to infer the model parameters which caused the observations—an inverse problem. Bayesian inference can be used to express the solution to inverse problems in terms of a high-dimensional posterior distribution. Evaluating the mean or uncertainty of the posterior distribution involves the computation of high-dimensional integrals, which can be solved efficiently using, e.g., multilevel Monte Carlo or quasi-Monte Carlo methods. This special session brings together experts in the field to showcase some recent theoretical and computational contributions in the study of Bayesian inference using Monte Carlo and quasi-Monte Carlo methods.

- Laura Scarabosio*, “High-Dimensional Bayesian Level Set Inversion in Time-Domain Acoustic Waves” p. 134
- Max Orteu Capdevila*, “Fast Bayesian shape parameter estimation for parabolic PDEs in moving domains” p. 136
- Philipp A. Guth*, “Bayesian inference for output-feedback control of uncertain linear systems” p. 138
- Charlotte Lämblgen*, “A Novel Convolutional Path Approach for Sampling with Interacting Particle Systems” p. 139

Friday June 12th, 10:30 – 12:30, JCMB Lecture Theatre A

Stochastic computation and complexity, Part 5

Organizers:

Stefan Heinrich
RPTU, University Kaiserslautern
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Session Description:

The session is devoted to algorithms and complexity for quadrature of SDEs and SPDEs, in particular under nonstandard assumptions, approximation of stochastic processes, high and infinite dimensional integration and approximation, including aspects of lower bounds and connections to functional analysis and stochastic analysis.

- David Krieg*, “A construction for optimal least squares approximation” p. 147
- Kateryna Pozharska*, “Function discretization and related questions” p. 149
- Nicolas Nagel*, “Precise asymptotics and exact expressions for QMC-errors of Fibonacci lattices” p. 152
- Marcin Wnuk*, “Regularizing the randomized QMC quadratures via the Median of Means.” p. 154

Friday June 12th, 10:30 – 12:30, JCMB Lecture Theatre B

MCQMC for digital twins

Organizers:

Philipp A. Guth

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Vesa Kaarnioja

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Session Description:

André-Alexander Zepernick Freie Universität Berlin

Digital twins mirror physical systems to enable real-time monitoring, prediction, and control. In this context, the quantification of uncertainties in large-scale, model-based decision and optimization problems plays a central role. Uncertainties may arise from incomplete knowledge of material properties, boundary conditions, model parameters, or sensor configurations used to calibrate and update the digital twin. Addressing these challenges requires efficient methods for high-dimensional uncertainty propagation and inference, such as multilevel and quasi-Monte Carlo techniques, surrogate modeling, and Bayesian updating. This session will highlight recent advances in the computational and theoretical treatment of uncertainty quantification and data assimilation for digital twins, emphasizing their role in reliable prediction and control of complex systems.

Frances Y. Kuo, “Quasi-Monte Carlo for precision oncology – towards predictive digital twins” p. 147

Tapio Helin, “Efficient Entropy-Driven Strategies for Bayesian Optimal Experimental Design” p. 150

Robert Gruhlke, “A one-shot method for Bayesian optimal experimental design” p. 152

André-Alexander Zepernick, “From Flat to Curved: UQ for PDEs on Random Surfaces using QMC” p. 155

Friday June 12th, 10:30 – 12:30, JCMB Lecture Theatre C

Recent advances in hierarchical methods for uncertainty quantification, Part 2

Organizers:

Arved Bartuska

King Abdullah University of Science and Technology

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Yang Liu

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Session Description:

Quantifying uncertainties in models and applications typically involves numerical estimations of high-dimensional integrals. Monte Carlo (MC) methods provide a sample-based estimate that does not suffer from the curse of dimensionality. Quasi-MC (QMC) methods provide an approximation that converges faster under certain regularity conditions, typically at the expense of a dimension-dependent multiplicative term in the error. Hierarchical methods provide improvements in computational efficiency by harnessing trade-offs between different levels of accuracy of integrand approximations, making highly

accurate estimates feasible. This session explores recent advances in hierarchical MC and QMC methods and their applications.

Arved Bartuska, “Multilevel double-loop quasi-Monte Carlo methods for nested integration” p. 148

Matteo Raviola, “A function approximation algorithm using multilevel active subspaces” p. 150

Stjepan Salatović, “Multilevel Gaussian Processes with Applications to Inverse Problems” p. 153

M. Croci, “Level-set approximation of noisy functions” p. 155

Friday June 12th, 10:30 – 12:30, JCMB 5326

Monte Carlo Methods for Stochastic Reaction Networks

Organizers:

Chiheb Ben Hammouda

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Maksim Chupin

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Raúl Tempone

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Session Description:

Stochastic reaction networks (SRNs) are a class of continuous-time Markov chains widely used to model the time evolution of biological and chemical reactions, epidemics, and queuing networks. This special session focuses on recent advances in Monte Carlo methods for SRNs, including variance reduction techniques for rare-event estimation, analysis of model reduction on stochastic dynamics and information transfer, and simulation methods for non-Markovian reaction networks. The focus is on scalable algorithms and reliable uncertainty quantification for complex reaction networks.

David J. Warne, “Multifidelity simulation and inference methods for non-Markovian reaction networks” p. 149

Juan David Marmolejo Lozano, “Effects of Model Reduction on Coherence and Information Transfer in Stochastic Biochemical Systems” p. 151

Maksim Chupin, “Tensor Train Decomposition for Optimal Importance Sampling in Stochastic Reaction Networks” p. 153

Abstracts

Monday June 8th – Afternoon/1, 15:30 – 16:00, JCMB Lecture Theatre A

Strong convergence rates for a Lie-Trotter splitting scheme for the CIR process

Session: Stochastic computation and complexity, Part 1

p. 35

Andreas Neuenkirch

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We study the strong approximation of the Cox-Ingersoll-Ross (CIR) process by means of a Lie-Trotter splitting, which separates the CIR process into a linear ordinary differential equation and the stochastic differential equation (SDE) of the squared Bessel process. Similar splitting approaches have been studied for the weak approximation of the CIR process, see e.g. [1,2], but not yet for strong approximation.

If the Feller index of the CIR process satisfies $\nu > 1/2$, then our method attains for all $\epsilon > 0$ an L^1 -error in the discretization points of order $\min\{1, \nu\} - \epsilon$ in terms of the maximal step size of the discretization.

Our Lie-Trotter splitting scheme is implementable, since the squared Bessel SDE can be explicitly solved in terms of the driving Brownian motion and its running infimum, see e.g. [3]. The joint distribution of the latter can be simulated exactly, see e.g. [4]. Additionally, the exact simulation of the squared Bessel process can be replaced by its approximation from [3], which uses adaptive evaluations of the driving Brownian motion only. The overall convergence order remains unchanged, and in this way we obtain a new upper for the minimal error for the L^1 -approximation of the CIR process at a single point by methods which rely on the point evaluation of Brownian motion.

- [1] Ninomiya, S., Victoir, N. (2008). Weak approximation of stochastic differential equations and application to derivative pricing. *Appl. Math. Finance* 15(2), 107-121.
- [2] Alfonsi, A. (2010). High order discretization schemes for the CIR process: application to affine term structure and Heston models. *Math. Comput.* 79(269), 209-237.
- [3] Hefter, M., Herzwurm, A. (2017). Optimal strong approximation of the one-dimensional squared Bessel process. *Commun. Math. Sci.* 15(8), 2121-2141.
- [4] Lépingle, D. (1995). Euler scheme for reflected stochastic differential equations. *Math. Comput. Simul.* 38(1-3), 119-126.

Monday June 8th – Afternoon/1, 15:30 – 16:00, JCMB Lecture Theatre B

Efficient Sampling of Extreme Heatwaves and Rainfall in an Intermediate-Complexity Climate Model

Session: Rare event simulation for quantifying climate uncertainties: theory and practice p. 35

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Coauthor(s): Freddy Bouchet, Francesco Ragone, Reinhard Schiemann, Len Shaffrey

Climate change is increasing the frequency and severity of extreme events such as floods, heatwaves, and droughts. To assess future risks, climate researchers often use numerical models to simulate the evolution of the atmosphere, oceans and other Earth system components. Yet, achieving the spatial resolution necessary to capture the underlying turbulent processes makes these simulations computationally expensive, especially when large samples are needed to study rare extremes.

Rare-event simulation techniques, such as genealogical particle analysis and multilevel splitting, offer a powerful way to accelerate the sampling of such events. In this talk, I will discuss how such methods have been applied to the intermediate-complexity climate model PlaSim. I will highlight results demonstrating that genealogical particle analysis can significantly speed up the exploration of extreme European summer heatwaves and winter rainfall events, enabling more efficient and targeted analysis of high-impact climate extremes.

Monday June 8th – Afternoon/1, 15:30 – 16:00, JCMB Lecture Theatre C

Slice Sampling using Approximations

Session: Advances in slice sampling and related methodologies p. 36

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Slice sampling is a well-established Markov chain Monte Carlo method for drawing (approximate) samples from a posterior distribution that is often known only up to a normalizing constant. The method is based on choosing a new state on a slice, i.e., a superlevel set of the (unnormalized) target density with respect to a reference measure. However, slice sampling algorithms typically require multiple evaluations of the target density per iteration and can therefore become computationally expensive, particularly in high-dimensional settings. To mitigate these costs, in this talk we examine how deterministic approximations of the target density can be incorporated into slice sampling schemes. We demonstrate the effectiveness of our methods with several numerical experiments in the context of Bayesian inference.

Monday June 8th – Afternoon/1, 15:30 – 16:00, JCMB 5326

Structurally-informed diffusion modeling

Session: Markov operators for data generation and inference based on denoising diffusions p. 37

Zheyang Shen

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Coauthor(s): Huihui Wang, Marina Riabiz, Chris Oates

The empirical success of diffusion models underscores the effectiveness of distributional approximation via the learned reverse process, which acts as a surrogate mirroring the noising dynamics. Despite the largely black-box nature of this approximation, the noising processes themselves are mathematically well understood, as they perform the comparatively simple task of “creating noise from data”.

The asymmetry between a well-understood, principled noising process and its black-box, learned time reversal lays the groundwork for the central question of this talk:

As the reverse process is expected to emulate the noising dynamics backward in time, what insights arising from the *structural constraints* of the forward noising process can be extracted to facilitate learning and inference in diffusion models?

This talk discusses the incorporation of such structural constraints for better-informed score matching in score-based generative models. Notably, we illustrate that it is possible to (i) reformulate the implicit score matching loss of Hyvärinen from an *operator-centric* viewpoint and (ii) obtain training-free parametric score estimates for all noise levels, using only sample averages with respect to the data distribution. The resulting *operator-informed score matching* provides both a standalone approach to sample generation for low-dimensional distributions, as well as a recipe for aiding the training of neural score estimators in practical high-dimensional settings.

Monday June 8th – Afternoon/1, 16:00 – 16:30, JCMB Lecture Theatre A

On Tamed Euler Schemes for Multidimensional SDEs with a Discontinuous Drift Coefficient

Session: Stochastic computation and complexity, Part 1 p. 35

Christopher Rauhögger

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Coauthor(s): T. Johnston, T. Müller-Gronbach, S. Sabanis, L. Yaroslavtseva

Existence, uniqueness, and L_p -approximation results are presented for autonomous d -dimensional systems of stochastic differential equations in the case where the drift coefficient μ may have discontinuities and where both coefficients can grow superlinearly.

To be more precise, we assume that there exists a compact C^4 -hypersurface $\Theta \subseteq \mathbb{R}^d$ such that μ is locally intrinsic Lipschitz continuous on $\mathbb{R}^d \setminus \Theta$. Furthermore, the diffusion coefficient σ is assumed to be locally Lipschitz continuous and has a non-degenerate portion orthogonal to Θ . Finally, it is assumed that the local (intrinsic) Lipschitz constants

of μ and σ grow at most polynomially and that μ and σ fulfill a monotonicity condition on $\mathbb{R}^d \setminus \Theta$ as well as a global coercivity condition.

Monday June 8th – Afternoon/1, 16:00 – 16:30, JCMB Lecture Theatre B

Rare event sampling of Arctic sea ice reduction and collapse of the Atlantic Meridional Overturning Circulation

Session: Rare event simulation for quantifying climate uncertainties: theory and practice p. 35

Francesco Ragone

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Extreme events like heat waves, floods or wind storms, as well as abrupt transitions associated with tipping elements of the climate system, can have severe impacts on human societies and ecosystems. Studying these events on a robust statistical basis is challenging, as only few events (if any) are available in observational data, and running numerical models for long enough in order to sample a sufficient number of them is usually computationally prohibitive. A possible approach to overcome these issues is given by rare event algorithms, computational techniques designed to oversample model trajectories leading to target rare events of interest, allowing to compute their probability with reasonable uncertainties and helping identifying their dynamical drivers. We will discuss in general the challenges we face when dealing with rare extreme events and abrupt transitions in the climate system and how rare event sampling techniques can help overcome them. We will then discuss applications of these techniques to events involving the coupled atmosphere-ocean-cryosphere system, focusing on extremes of Arctic sea ice reduction and on abrupt transitions associated with the weakening and collapse of the Atlantic Meridional Overturning Circulation.

Monday June 8th – Afternoon/1, 16:00 – 16:30, JCMB Lecture Theatre C

Advances in Stereographic Slice Sampling

Session: Advances in slice sampling and related methodologies p. 36

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Coauthor(s): Krzysztof Łatuszyński and Gareth Roberts

Stereographic MCMC algorithms [1,2] use the stereographic projection to improve the convergence properties of Markov chain Monte Carlo algorithms, particularly for high-dimensional, heavy-tailed sampling problems. The projection works by mapping \mathbb{R}^d onto the unit d -sphere \mathbb{S}^d , which is compact. When targeting isotropic distributions, we obtain a blessing of dimensionality wherein convergence properties of our algorithms do not decay as the dimension of the problem increases. The best-performing algorithm among those discussed has been found to be the stereographic slice sampler [2].

The closer the projection of the target density onto \mathbb{S}^d is to a uniform distribution, the better the sampling properties of the algorithm. For the most part, this can be addressed using an affine preconditioner. However, in the presence of skewness or extremely

heavy tails, such a preconditioning may not be sufficient to remove certain problematic behaviours. To address these, the sub-Cauchy sampler [3] was introduced using an extension of the stereographic projection, but only in the context of random-walk Metropolis algorithms. In this talk, we generalise the stereographic slice sampler to the novel sub-Cauchy slice sampler. We provide theoretical and empirical results to compare its performance against other algorithms.

- [1] Bell, C., Łatuszyński, K., & Roberts, G. O. (2025). *Adaptive Stereographic MCMC*. ArXiv.org. <https://arxiv.org/abs/2408.11780>
- [2] Yang, J., Łatuszyński, K., & Roberts, G. O. (2024). Stereographic Markov chain Monte Carlo. *The Annals of Statistics*, 52(6). <https://doi.org/10.1214/24-aos2426>
- [3] Grazi, S., Liu, S., Roberts, G. O., & Yang, J. (2026). *Sub-Cauchy Sampling: Escaping the Dark Side of the Moon*. ArXiv.org. <https://arxiv.org/abs/2601.11066>

Monday June 8th – Afternoon/1, 16:00 – 16:30, JCMB 5326

Operator-informed control variates for denoising diffusion samplers

Session: Markov operators for data generation and inference based on denoising diffusions
p. 37

Huihui Wang

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Coauthor(s): Zheyang Shen, Marina Riabiz, Chris Oates

Ideas from denoising diffusion models (DDMs) [1] have been increasingly adopted in the design of algorithms for sampling from unnormalized distributions, including the variational approach of denoising diffusion samplers (DDSs) [2]. However, the variance of the resulting estimators is generally not guaranteed to be low. Control variates are a widely used variance reduction technique in sampling. Motivated by operator-informed score matching for DDMs whose underlying dynamics is governed by a Markov diffusion process [3], we develop operator-based control variates for DDSs. Comprehensive experimental results demonstrate that the proposed method effectively reduces the variance of samples produced by DDSs.

[1] Song, Y., Sohl-Dickstein, J., Kingma, D.P., Kumar, A., Ermon, S., and Poole, B. Score-Based Generative Modeling through Stochastic Differential Equations. In *Proceedings of the 8th International Conference on Learning Representations*, 2020.

[2] Vargas, F., Grathwohl, W. and Doucet, A., 2023. Denoising diffusion samplers. arXiv preprint arXiv:2302.13834.

[3] Shen, Z., Wang, H., Riabiz, M. and Oates, C.J., 2024. Operator-informed score matching for Markov diffusion models. arXiv preprint arXiv:2406.09084.

Monday June 8th – Afternoon/1, 16:30 – 17:00, JCMB Lecture Theatre A

When Potentials Get Rough: Langevin & Diffusion Sampling in Semi-Convex Settings

Session: Stochastic computation and complexity, Part 1

p. 35

Sotirios Sabanis

University of Edinburgh, Archimedes/Athena Research Centre and NTU of Athens

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This talk explores recent progress in the challenging setting of semi-convex, non-smooth potentials, where classical smooth assumptions break down but rich structure remains. We develop a diffusive viewpoint that enables efficient sampling and detailed analysis in these rough energy landscapes, highlighting stability, convergence, and practical implementation. Applications illustrate how such stochastic methods remain effective even in the presence of irregularities and high-dimensional complexity.

Monday June 8th – Afternoon/1, 16:30 – 17:00, JCMB Lecture Theatre B

Estimation of the Variance Landscape in Multinomial Sequential Monte Carlo Sampling

Session: Rare event simulation for quantifying climate uncertainties: theory and practice

p. 35

Mathias Rousset

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Coauthor(s): Frédéric Cérou, Patrick Héas

Sequential Monte Carlo (SMC) is a standard sample-based simulation method for approximating target distributions known up to a normalization constant, such as those associated with rare events for a given Markov chain. A key challenge in SMC lies in the choice of importance functions, which steer the selection of individuals (a.k.a. “particles”) toward the prescribed rare event and strongly influence the method’s performance.

Building on previous work by Lee and Whiteley, and by Del Moral (with Patras, Cérou, Guyader, and others), we study *a posteriori* estimators of the output variance that can be computed at no additional cost via coalescence analysis. Our main contribution is a direct extension of these estimators — also at no extra cost — that enables the estimation of the variance for a range of SMC schemes constructed with nearby but distinct parameter choices, in particular different importance functions.

We establish unbiasedness and provide an L^2 error analysis. Applications to the optimisation of importance functions will be discussed in the talk by P. Héas in the same mini-symposium.

Monday June 8th – Afternoon/1, 16:30 – 17:00, JCMB Lecture Theatre C

Geodesic Slice Sampler for Multimodal Distributions with Strong Curvature

Session: Advances in slice sampling and related methodologies p. 36

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Traditional Markov Chain Monte Carlo methods often struggle in the presence of strong curvature, complex geometry, and multimodality. Slice sampling improves local exploration, while Riemannian approaches adapt proposals to the geometry of the target distribution. Recent work on geodesic slice sampling on Riemannian manifolds [1] shows that leveraging closed-form geodesics can extend hit-and-run slice sampling to more general geometries, but is limited to settings where such geodesics are available.

In this talk, we present a geodesic slice sampler for highly curved and multimodal distributions in Euclidean space. Our approach introduces suitable Riemannian metrics and approximates geodesics as solutions to differential equations, removing the need for closed-form solutions. This yields a hit-and-run-style sampler that follows the local geometry of the target distribution, enabling efficient exploration of regions with strong curvature and improved transitions between modes. We demonstrate its advantages on a range of sampling problems.

- [1] Durmus, A., Gruffaz, S., Hasenpflug, M., and Rudolf, D. (2026). Geodesic slice sampling on Riemannian manifolds. *Biometrika*, asag006.

Monday June 8th – Afternoon/1, 16:30 – 17:00, JCMB 5326

Generator-based Graph Generation via Heat Diffusion

Session: Markov operators for data generation and inference based on denoising diffusions p. 37

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Graph generative modelling has become an essential task due to the wide range of applications in chemistry, biology, social networks, and knowledge representation. In this work, we propose a novel framework for generating graphs by learning a surrogate of the Markov generator of the graph noising process. We leverage the graph Laplacian and its associated heat kernel to define a continuous-time diffusion on a graph. The Laplacian serves as the infinitesimal generator of this diffusion, and its heat kernel provides a family of conditional perturbations of the initial graph. A neural network is trained to match this generator by minimising a Bregman divergence between the true generator and a learnable surrogate. Once trained, the surrogate generator is used to simulate a time-reversed diffusion process to sample new graph structures. Our framework unifies and

generalises existing diffusion-based graph generative models, injecting domain-specific inductive bias via the Laplacian, while retaining the flexibility of neural approximators. Experimental studies demonstrate that our approach captures structural properties of real and synthetic graphs effectively.

Monday June 8th – Afternoon/1, 17:00 – 17:30, JCMB Lecture Theatre A

Itô perspective on variance renormalisation

Session: Stochastic computation and complexity, Part 1

p. 35

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We show that the Itô solutions of the nonlinear stochastic heat equation

$$\partial_t u^\varepsilon - \Delta u^\varepsilon = \varepsilon^{3/4} g(u^\varepsilon) \nabla \xi_\varepsilon,$$

where ξ_ε denotes the mollification in space at scale $\varepsilon > 0$ of a space-time white noise ξ , converge in law, as $\varepsilon \rightarrow 0$, to the solution of the stochastic heat equation with right-hand side $cg'g(u)\xi$ with a constant $c > 0$. Since the noise $\nabla \xi$ is supercritical, the small prefactor is not unexpected to obtain a limit, but the exponent $3/4$ is not predicted by naive scaling arguments. The case $g(u) = u$, modulo a Cole–Hopf transform, corresponds to the result of Hairer (2025) for the KPZ equation. Our argument is relatively short and relies solely on stochastic analytic techniques.

Monday June 8th – Afternoon/1, 17:00 – 17:30, JCMB Lecture Theatre B

Numerical study of a variance optimisation algorithm in sequential Monte-Carlo

Session: Rare event simulation for quantifying climate uncertainties: theory and practice

p. 35

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This work focuses on reducing the variance of estimators computed using sequential Monte Carlo (SMC) with multinomial resampling. Assuming that the importance functions belong to a parametric family, the main idea is to minimize the asymptotic variance of the SMC estimator by optimizing these functions. Specifically, this work first demonstrates how to construct an unbiased and consistent estimator of the derivative of the asymptotic variance with respect to the parameter of the importance functions. This estimator is based on the SMC genealogical tree and one-coalescence plans within the tree. The second contribution is proposing an algorithm of linear complexity to compute this estimator. Third, we propose an optimization scheme based on a stochastic gradient algorithm to estimate the local minimizer of the asymptotic variance. Finally, we demonstrate the consistency of the derivative estimator and the convergence of the

stochastic gradient algorithm to the variance minimizer using Ornstein-Uhlenbeck processes. We also empirically demonstrate variance reduction for other types of processes using state-of-the-art parametric families of importance functions.

Monday June 8th – Afternoon/1, 17:00 – 17:30, JCMB Lecture Theatre C

Spectral gap of uniform and geodesic slice sampling on the sphere

Session: Advances in slice sampling and related methodologies

p. 36

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Geodesic slice sampling on the sphere (GSSS) [1] was recently developed as a general purpose MCMC method for targeting intractable distributions on the Euclidean d -sphere \mathbb{S}^d . Numerical experiments show GSSS to be fairly robust under challenging properties of the target distribution, such as high dimensions, complicated geometries and even multi-modality.

On the other hand, our understanding of how the performance of GSSS is affected by the target distribution’s concentration (including its tail type) is still quite limited: At one extreme, for targets that are tightly concentrated around a single point, intuitive arguments suggest that the performance of GSSS should exhibit a moderate dimension-dependence. On the other end of the spectrum, for the target being the uniform distribution on all of \mathbb{S}^d , GSSS has been shown to maintain a certain baseline performance independent of the dimension [2]. Since most realistic applications of GSSS would fall somewhere in between these two extremes, it is of significant practical interest how well the method performs in this intermediate regime.

We aim to illuminate this topic by analyzing the performance of GSSS, as quantified by the L_2 -spectral gap of its induced linear operator, through that of the underlying idealized method, uniform slice sampling on the sphere (USSS), using the Poincaré inequality framework of [3]. Our goal is to derive performance guarantees in the form of “scaling laws” that provide lower bounds on the spectral gaps of USSS and GSSS, depending on the target distribution’s concentration and tail type parameters.

- [1] Michael Habeck, Mareike Hasenpflug, Shantanu Kodgirwar & Daniel Rudolf. *Geodesic slice sampling on the sphere*. Journal of Machine Learning Research 26(297), 2025.
- [2] Philip Schär & Thilo Stier. *A dimension-independent bound on the Wasserstein contraction rate of a geodesic random walk on the sphere*. Electronic Communications in Probability 29(62), 2024.
- [3] Sam Power, Daniel Rudolf, Björn Sprungk & Andi Q. Wang. *Weak Poincaré inequality comparisons for ideal and hybrid slice sampling*. arXiv:2402.13678v2, 2025.

Monday June 8th – Afternoon/2, 15:30 – 16:00, JCMB 5327

Tuning-Free Sampling via Optimization on the Space of Probability Measures

Session: Gradient Flow for Sampling

p. 38

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We introduce adaptive, tuning-free step size schedules for gradient-based sampling algorithms obtained as time-discretizations of Wasserstein gradient flows. The result is a suite of tuning-free sampling algorithms, including tuning-free variants of the unadjusted Langevin algorithm (ULA), stochastic gradient Langevin dynamics (SGLD), mean-field Langevin dynamics (MFLD), Stein variational gradient descent (SVGD), and variational gradient descent (VGD). More widely, our approach yields tuning-free algorithms for solving a broad class of stochastic optimization problems over the space of probability measures. Under mild assumptions (e.g., geodesic convexity and locally bounded stochastic gradients), we establish strong theoretical guarantees for our approach. In particular, we recover the convergence rate of optimally tuned versions of these algorithms up to logarithmic factors, in both nonsmooth and smooth settings. We then benchmark the performance of our methods against comparable existing approaches. Across a variety of tasks, our algorithms achieve similar performance to the optimal performance of existing algorithms, with no need to tune a step size parameter.

Monday June 8th – Afternoon/2, 15:30 – 16:00, JCMB 5328

Structural Properties of Multiply-with-Carry Random Number Generators

Session: Point Sets and Distributions

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Random number generators based on a multiple linear recurrence with carry, aka multiply-with-carry (MWC), were proposed by Marsaglia over 30 years ago [1]. These generators are very fast, because using a carry in the recurrence permits one to use arithmetic modulo a power of 2 and still obtain a very long period. Unfortunately, the specific instances proposed by Marsaglia at the time had major defects in their structure and multivariate uniformity [2], and have been mostly discarded long ago. Different instances proposed in [3] also had defects, as shown in [4]. In this talk, we show how to construct reliable MWC generators that can produce up to two billion 64-bit uniform random numbers per second on a laptop computer with a single CPU. The quality of these generators is assessed by a mathematical analysis of their multivariate structure. We also have new theoretical results regarding the lattice structure of these types of generators.

[1] G. Marsaglia. 1994. Yet Another RNG. <https://groups.google.com/g/sci.stat.math/c/p7aLW3TsJys?pli=1>, August 1, 1994.

[2] R. Couture and P. L'Ecuyer. Distribution Properties of Multiply-with-Carry Random Number Generators. *Mathematics of Computation* 66, 218 (1997), 591–607.

[3] M. Goresky and A. Klapper. Efficient Multiply-with-Carry Random Number Generators with Maximal Period. *ACM Transactions on Modeling and Computer Simulation* 13, 4 (2003), 310–321.

[4] P. L'Ecuyer. Fast and Reliable Multiply-With-Carry Random Number Generators. Forthcoming, 2026.

Monday June 8th – Afternoon/2, 15:30 – 16:00, JCMB 6206

On the forgetting of particle filters

Session: Particle Methods

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We study the forgetting properties of the particle filter when its state — the collection of particles — is regarded as a Markov chain. Under a strong mixing assumption on the particle filter's underlying Feynman–Kac model, we find that the particle filter is exponentially mixing, and forgets its initial state in $O(\log N)$ ‘time’, where N is the number of particles and time refers to the number of particle filter algorithm steps, each comprising a selection (or resampling) and mutation (or prediction) operation. We present an example which shows that this rate is optimal. We also establish new propagation of chaos type results using our proof techniques. Our forgetting result extends relatively directly to the conditional particle filter (CPF), once we establish new time-uniform L^p error estimates for CPF, which can be of independent interest. The talk is based on the article [1].

[1] Joonas Karjalainen, Anthony Lee, Sumeetpal S. Singh and Matti Vihola. *On the forgetting of particle filters*, arXiv:2309.08517. <https://arxiv.org/abs/2309.08517>

Monday June 8th – Afternoon/2, 16:00 – 16:30, JCMB 5327

A gradient flow interpretation of sequential Monte Carlo

Session: Gradient Flow for Sampling

p. 38

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We consider the problem of sampling from a probability distribution π . It is well known that this can be written as an optimisation problem over the space of probability distribution in which we aim to minimise the Kullback–Leibler divergence from π . This talk will highlight recent connections between gradient flows in the Fisher–Rao and Wasserstein–Fisher–Rao geometry and sequential Monte Carlo methods. We will highlight how the gradient flow interpretation gives a natural way to compare importance

sampling based algorithms with classical Markov chain Monte Carlo algorithms as the unadjusted Langevin algorithm.

[1] Nicolas Chopin, Francesca Crucinio, and Anna Korba. *A connection between tempering and entropic mirror descent*. In Ruslan Salakhutdinov, Zico Kolter, Katherine Heller, Adrian Weller, Nuria Oliver, Jonathan Scarlett, and Felix Berkenkamp, editors, Proceedings of the 41st International Conference on Machine Learning, volume 235 of Proceedings of Machine Learning Research, pages 8782–8800. PMLR, 21–27 Jul 2024

[2] Francesca R. Crucinio and Sahani Pathiraja. *Sequential Monte Carlo approximations of Wasserstein–Fisher–Rao gradient flows*. arXiv preprint arXiv: 2506.05905, 2025.

Monday June 8th – Afternoon/2, 16:00 – 16:30, JCMB 5328

Extended SZ Sequences

Session: Point Sets and Distributions

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SZ sequences are a recently introduced family of $(0, 2^q)$ -sequences in base 2^q , constructed from binary $\text{GF}(2)$ matrices. These matrices are built from sets of $q \times q$ blocks that satisfy the algebraic properties of $\text{GF}(2^q)$.

We show that this block-based construction conforms to Niederreiter’s digital construction framework and, accordingly, that the resulting SZ sequences implement Niederreiter’s extension of Faure sequences, as previously conjectured by the authors. However, this formulation additionally exposes the nested substructure of these sequences.

We discuss the existence of this empirically developed SZ construction by relating admissible block-matrix sets to primitive polynomials over $\text{GF}(2)$. We then show that each $(0, 2^q)$ SZ sequence can be extended to arbitrary dimension by implementing the Faure–Lemieux irreducible Sobol construction, thereby placing Sobol and SZ sequences within a unified construction framework.

Finally, we propose a dimension-dependent base selection map identifying which base may be preferable for a given dimension, based on comparisons of the dyadic quality factor t .

[1] Abdalla G. M. Ahmed, Matt Pharr, Victor Ostromoukhov, and Hui Huang. 2025. SZ Sequences: Binary-Based $(0, 2^q)$ -Sequences. ACM Trans. Graph. 44, 6, Article 206 (December 2025), 14 pages. <https://doi.org/10.1145/3763272>

Monday June 8th – Afternoon/2, 16:00 – 16:30, JCMB 6206

Robust, partially alive particle Metropolis-Hastings via the Frankfilter

Session: Particle Methods

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When a hidden Markov model permits the conditional likelihood of an observation given the hidden process to be zero, all particle simulations from one observation time to the next could produce zeros. If so, the filtering distribution cannot be estimated and the estimated parameter likelihood is zero. The alive particle filter addresses this by simulating a random number of particles for each inter-observation interval, stopping after a target number of non-zero conditional likelihoods. For outlying observations or poor parameter values, a non-zero result can be extremely unlikely, and computational costs prohibitive. We introduce the Frankenfilter, a principled, partially alive particle filter that targets a user-defined amount of success whilst fixing lower and upper bounds on the number of simulations. The Frankenfilter produces unbiased estimators of the likelihood, suitable for pseudo-marginal Metropolis–Hastings (PMMH). We demonstrate that PMMH with the Frankenfilter is more robust to outliers and mis-specified initial parameter values than PMMH using standard particle filters, and is typically at least 2-3 times more efficient. We also provide advice for choosing the amount of success. In the case of n exact observations, this is particularly simple: target n successes.

Monday June 8th – Afternoon/2, 16:30 – 17:00, JCMB 5327

Maximum marginal likelihood, EM, Gradient flows and a log-Sobolev inequality

Session: Gradient Flow for Sampling

p. 38

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Maximum marginal likelihood estimation and Empirical Bayes are fundamental procedures in statistics and machine learning. They arise, for instance, in parameter inference problems within state-space models, probabilistic principal component analysis, missing data problems, and more. First, we will discuss various algorithms for tackling this estimation problem, which implement various optimization strategies on the free energy functional (i.e. minus ELBO). These include, among others, the EM algorithm and some gradient flows methods recently introduced in the literature. Then, we will introduce a fundamental functional inequality that characterizes the fast convergence of all these algorithms. We will see how this inequality generalizes upon the log-Sobolev and Polyak–Łojasiewicz inequalities, establishing connections with various concepts and results in optimal transport.

Monday June 8th – Afternoon/2, 16:30 – 17:00, JCMB 5328

A dice game, a multinomial walk, and the inverted Dirichlet distribution

Session: Point Sets and Distributions

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We consider a simple dice game, which leads to an intriguing study of multinomial walks, with surprising and seemingly paradoxical properties. The winning and losing probabilities of a general version of the game are investigated via conjugacy relations between Gamma and Poisson distributions, as well as between negative multinomial and inverted Dirichlet distributions. We show a monotonicity property of the regularized beta function, which implies a monotonicity property of the winning probability. Furthermore, the asymptotic behavior of the game for one or several parameters of the game tending to infinity is analyzed, as well as the probability of being last in the game.

Monday June 8th – Afternoon/2, 16:30 – 17:00, JCMB 6206

Aspects of Generalized Bayesian Inference in Ensemble and Particle Filters

Session: Particle Methods

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Recent advances in generalized Bayesian inference and corresponding generalized posteriors offer novel opportunities for Bayesian data assimilation schemes such as the family of ensemble Kalman and particle filters. Appropriate choices of discrepancy measures allow deriving varieties of the celebrated Kalman filter with novel, desirable properties while maintaining Gaussian prior-likelihood conjugacy in the analysis step and stability under mild assumptions. This encourages investigating generalizations to more sophisticated and state-of-the-art approaches in data assimilation, e.g. stochastic EnKFs and the popular local ensemble transform Kalman filter (LETKF). Similarly, particle filters may be adjusted to obtain additional desirable properties yet maintain consistency in the particle limit without a relevant increase in computational budget. We will present some results and lessons learned from adaptations of EnKFs, LETKFs and particle filters in popular non-linear dynamical systems for study of behaviour and properties. A central focus will be the use of diffusion score matching (DSM) to capture discrepancy between measures of observation distributions with an appropriate choice of diffusion matrix to assimilate observations online under suspicion of mis-specification of the observation likelihood. The talk aims to provide a bird-eye view on the potentials and limitations of generalized Bayesian inference for Bayesian filtering and data assimilation.

Monday June 8th – Afternoon/2, 17:00 – 17:30, JCMB 5327

De-biased Simulation of the Mean Field Langevin Dynamics

Session: Gradient Flow for Sampling

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p. 38

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Amid increasing interest in formulating statistical inference as a nonlinear optimisation task, the limitations of existing numerical optimisation algorithms are becoming more pronounced. Numerical simulation of the mean field Langevin dynamics (MFLD), the foundation for many of the most popular algorithms, is intrinsically biased when a finite number of particles are used. To circumvent this challenge we present a novel debiasing strategy based on assigning weights that minimise the kernel gradient discrepancy in [1]. A key advantage of the proposed approach is that it can be applied purely as a post-processing step.

[1] C. Chazal, H. Kanagawa, Z. Shen, A. Korba, and C. J. Oates. *A computable measure of sub-optimality for entropy-regularised variational objectives*. arXiv:2509.10393, 2025.

Monday June 8th – Afternoon/2, 17:00 – 17:30, JCMB 6206

Mean shift interacting particles for unnormalized densities

Session: Particle Methods

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Approximating integrals with respect to unnormalized densities is a central task in Bayesian inference. Standard approaches, including MCMC and gradient-flow methods, often face substantial computational challenges in high dimensions. We introduce a class of interacting particle methods for numerical integration, based on a mean-shift dynamics that can be interpreted as a preconditioned gradient flow of a *symmetric* maximum mean discrepancy. By extending data-driven optimal quantization techniques to continuous measures, the resulting dynamics are invariant to the unknown normalizing constant of the target density, and admit both gradient-free and gradient-informed implementations. The resulting particle systems capture anisotropy and multimodality, avoid mode collapse, and remain effective in high-dimensional settings.

Tuesday June 9th – Morning/1, 10:30 – 11:00, JCMB Lecture Theatre A

Uniform approximation of infinite-variate functions from weighted Hilbert spaces

Session: Stochastic computation and complexity, Part 2

p. 39

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So far, the complexity of linear computational problems for infinite-variate functions has been mainly studied in a tensor product Hilbert space setting: The solution operator is a bounded linear operator of tensor product form between tensor product Hilbert

spaces H and G ; furthermore, H is a reproducing kernel Hilbert space. Examples include integration and L^2 -approximation (with respect to product probability measures) of functions from H .

In this talk, we study uniform approximation of functions from weighted Hilbert spaces, where we focus on product and order dependent weights.

Tuesday June 9th – Morning/1, 10:30 – 11:00, JCMB Lecture Theatre B

Curse of dimensionality vs. tractability for discrepancy – a survey

Session: Frontiers in QMC methods, Part 1 p. 39
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Coauthor(s): Erich Novak

There are different types of discrepancy with regard to different classes of test sets as well as with regard to different norms. In all cases, these are quantitative measures of the irregularity of the distribution of point sets, and often a discrepancy is related to the worst-case error of a quasi-Monte Carlo rule for the numerical integration of functions from suitable function spaces. Prominent examples are the star L_p discrepancy, the extreme L_p discrepancy, the periodic L_p discrepancy, the anchored L_p discrepancy, the quadrant (or centered) L_p discrepancy, and others. The inverse of a discrepancy for dimension d and error threshold $\varepsilon \in (0, 1)$ is the minimal number of points in $[0, 1]^d$ required such that the minimal discrepancy is less or equal an ε share of the initial discrepancy. For applications of QMC to high-dimensional problems, it is of great importance whether the inverse grows exponentially with the dimension (the curse of dimensionality) or not (tractability). Numerous authors have achieved many results in this area over the last three decades. Most of these concern L_2 and L_∞ discrepancies. The general L_p case remained elusive. Recently, together with Erich Novak, we developed a method that makes it possible to handle L_p discrepancies as well. In this talk, we present our method and some new results, and summarize all known results and open questions in a comprehensive overview.

Tuesday June 9th – Morning/1, 10:30 – 11:00, JCMB Lecture Theatre C

Neural Quasi-Monte Carlo

Session: Sampling and Machine Learning p. 40
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Low-discrepancy point sets are fundamental to efficient numerical integration and simulation, yet classical constructions based on number theory have remained largely

unchanged for decades. In this talk, I introduce Message-Passing Monte Carlo (MPMC), the first machine learning approach for generating low-discrepancy point sets, which leverages graph neural networks to achieve empirically optimal or near-optimal discrepancy, outperforming all classical constructions by a significant margin. I will discuss several extensions of this framework: to general non-uniform target distributions via a kernelized Stein discrepancy objective; to extensible low-discrepancy sequences via Neural Low-Discrepancy Sequences (NeuroLDS); and to a principled study of which discrepancy criteria are best suited to gradient-based optimization. Throughout, I demonstrate broad practical impact across quasi-Monte Carlo integration, scientific machine learning, and sampling-based robot motion planning.

Tuesday June 9th – Morning/1, 10:30 – 11:00, JCMB 5326

A Dynamic Perspective on Gaussian Processes and the Vanilla-SPDE Exchange

Session: Sampling and approximation for structured stochastic models in scientific computing, Part 1 p. 41

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Coauthor(s): Henry Moss, Lachlan Astfalck, Edward Cripps, David Leslie

Gaussian process (GP) models are widely used in statistics and machine learning, but are inherently static and treating observations as unordered, which lead to the cubic computational complexity. A dynamic perspective, available for a restricted class of GPs, reformulates their dependency structure unilaterally, enabling sequential inference with potentially linear computational scaling. Motivated by a practical spatio-temporal inference problem, we propose the Vanilla-SPDE Exchange (VaSE) framework that leverages the equivalence of the static and dynamic perspectives to synergise the computational benefits from both views. An application of VaSE for GP posterior sampling is described with cost analysis demonstrating noticeable computational speed-ups.

Tuesday June 9th – Morning/1, 11:00 – 11:30, JCMB Lecture Theatre A

Piecewise linear interpolation and the trapezoidal rule via kernels

Session: Stochastic computation and complexity, Part 2 p. 39

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We consider piecewise linear interpolation and the trapezoidal rule from the perspective of kernel interpolation and quadrature. If the Sobolev space $W_2^1(0, 1)$ is equipped with a suitable inner product, its reproducing kernel is piecewise linear and gives rise to piecewise linear interpolation. We show that such kernels are Green kernels for certain second-order partial differential equations and use kernel-based superconvergence theory to obtain rates of convergence for approximation of functions lying in $W_2^s(0, 1)$ for

$s \in [1, 2]$. The rates coincide with classical rates for linear splines. The talk is mostly based on the preprint [1].

[1] T. Karvonen, G. Santin & T. Wenzel (2026). Piecewise linear interpolation via kernels. *arXiv:2603.01555*.

Tuesday June 9th – Morning/1, 11:00 – 11:30, JCMB Lecture Theatre B

Uncertainty quantification using importance-sampled quasi-Monte Carlo with dimension-independent convergence rates

Session: Frontiers in QMC methods, Part 1

p. 39

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Quasi-Monte Carlo (QMC) integration over unbounded domains \mathbb{R}^s remains challenging due to the high dimensionality of sampling space and the boundary growth of the integrand. In applications such as uncertainty quantification (UQ), the dimension s can reach hundreds or even thousands. To restore the efficiency of quadrature rules in high dimensions, constructive QMC methods like lattice rules have been successfully developed within the framework of weighted function spaces. In contrast to designing problem-specific quadrature points, this paper proposes transforming the underlying integrand to accommodate the off-the-shelf scrambled nets (a construction-free randomized QMC method) via the boundary-damping importance sampling (BDIS) proposed by [1]. We provide a rigorous analysis of the dimension-independent convergence rate of BDIS-based scrambled nets while covering a broader class of unbounded functions than that in [1]. By exploiting the dimension structure of the parametric input random field, the proposed n -point quadrature rule achieves a dimension-independent mean squared error rate of $O(n^{-1-\alpha^*+\varepsilon})$ on standard UQ problems in elliptic partial differential equations (PDEs), where $\varepsilon > 0$ is arbitrarily small and $\alpha^* \in (0, 1)$ reflects the regularity with respect to the parametric variables. Numerical experiments on elliptic PDEs with high-dimensional parameters further demonstrate the effectiveness of the method.

[1] Pan, Z., Ouyang, D., and He, Z. (2025). Quasi-Monte Carlo integration over \mathbb{R}^s with boundary-damping importance sampling. *arXiv:2509.07509*, preprint.

Tuesday June 9th – Morning/1, 11:00 – 11:30, JCMB Lecture Theatre C

Almost nearly perfect Bayesian imaging with physics-informed deep generative models

Session: Sampling and Machine Learning

p. 40

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his talk introduces a novel mathematical and computational framework for constructing high-dimensional Bayesian inversion methods that leverage state-of-the-art generative

denoising diffusion models as highly informative priors. A central innovation is the use of Langevin diffusion processes and Markov chain Monte Carlo sampling techniques to create stochastic neural network architectures that perform nearly-perfect sampling. The obtained networks are modular and composed of interpretable layers that are directly related to statistical image priors and data likelihoods. The layers encoding the data likelihood function are designed for flexibility, enabling observation model parameters to be specified at inference time and seamlessly integrated with pre-trained foundational generative priors. To achieve high computational efficiency, we employ adversarial model distillation, which yields excellent sampling performance with as few as four Markov chain Monte Carlo steps, even in problems exceeding one million dimensions. Our approach is validated through non-asymptotic convergence analysis and extensive numerical experiments in computational image and video restoration. The talk is based on recent work in physics-informed generative AI for Bayesian imaging [1,2], which uses a distilled latent Stable Diffusion XL model trained on five billion clean images as a zero-shot prior; and [3], which integrates pixel-based diffusion models with deep unfolding and diffusion distillation.

[1] A. Spagnoletti, J. Prost, A. Almansa, N. Papadakis and M. Pereyra, LATINO-PRO: LAtent consisTency INverse sOlver with PRompt Optimization, in Proceedings of the International Conference on Computer Vision (ICCV), 2025. <https://latino-pro.github.io>

[2] A. Spagnoletti, A. Almansa, and M. Pereyra, LVTINO: LAtent Video consisTency INverse sOlver for High Definition Video Restoration, in Proceedings of the International Conference on Learning Representations (ICLR), 2026. <https://github.com/LATINO-PRO/LVTINO>

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Tuesday June 9th – Morning/1, 11:00 – 11:30, JCMB 5326

Accelerating posterior sampling in Bayesian inverse problems with score-based diffusion models

Session: Sampling and approximation for structured stochastic models in scientific computing, Part 1 p. 41

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The Bayesian approach offers a natural framework for uncertainty quantification in many high- and infinite-dimensional inverse problems. Their practical use is however often limited by the cost of posterior sampling. This difficulty is particularly severe in large-scale inverse problems, where standard MCMC methods can become prohibitively slow. In this talk, I will describe recent work on accelerating Bayesian nonparametric inverse problems using score-based diffusion models. A particular emphasis will be on the UCoS framework, where we introduce an *Unconditional representation of Conditional*

Score functions for infinite-dimensional linear inverse problems. This representation enables task-dependent training of diffusion models, leading to fast posterior samplers that avoid repeated evaluations of the forward operator while remaining consistent with the underlying Bayesian posterior. The validity of the method will be tested on different inverse problem applications, including CT imaging and deblurring.

Tuesday June 9th – Morning/1, 11:30 – 12:00, JCMB Lecture Theatre A

On the quantum complexity of parametric integration in Sobolev spaces

Session: Stochastic computation and complexity, Part 2

p. 39

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This talk is concerned with the quantum setting of Information-Based Complexity (IBC). We continue the study 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 $D = [0, 1]^d = D_1 \times D_2$, $D_1 = [0, 1]^{d_1}$, $D_2 = [0, 1]^{d_2}$. What makes this problem interesting for IBC is that it is intermediate between integration ($d_1 = 0$) and approximation ($d_2 = 0$). Under the assumption that $W_p^r(D)$ is embedded into $C(D)$ (embedding condition) the case $p = q$ was partially solved by Wiegand [1] (for $1 \leq p < \infty$, $r > 2d_1 + d_2$). Here we present some generalizations to the case $p = q$ without embedding condition and to the general case $p \neq q$ with or without the embedding condition. We compare the rates with those in the (classical) randomized setting [2]. In contrast to the essentially complete picture of [2], in the quantum setting many cases remain open, which will also be discussed.

[1] Wiegand, Carsten (2006). *Optimal Monte Carlo and Quantum Algorithms for Parametric Integration*. Shaker Verlag.

[2] Heinrich, Stefan (2024). Randomized complexity of parametric integration and the role of adaption II. Sobolev spaces. *Journal of Complexity* 82, 101823.

Tuesday June 9th – Morning/1, 11:30 – 12:00, JCMB Lecture Theatre B

The L_p approximation using multiple lattice based algorithm

Session: Frontiers in QMC methods, Part 1

p. 39

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In this talk, we study the approximation of periodic functions on the d -dimensional unit cube $[0, 1]^d$ in the weighted Korobov spaces $H_{d,\alpha,\gamma}$. A popular method is the single lattice-based algorithm, which approximates $f \in H_{d,\alpha,\gamma}$ by combining the truncated

Fourier series on the index set \mathcal{A}_d with the discretization of the coefficients $\hat{f}(\mathbf{k})$ using a rank-1 lattice rule. However, a single rank-1 lattice invariably suffers from aliasing issues and fails to achieve the optimal convergence rate. To overcome this, a reconstruction strategy using a union of rank-1 lattices was proposed by Kämmerer. Despite these advances, the optimality of the L_2 error (or its randomized version) for multiple lattice-based algorithms has not been fully explored in this weighted setting. We bridge this gap by proving that for any smoothness parameter $\alpha > 1/2$, the multiple lattice-based algorithm attains a nearly optimal convergence rate for the worst-case L_∞ error. Furthermore, when incorporating random shifts, these algorithms achieve a nearly optimal convergence rate for the worst-case root mean squared L_2 error. Finally, we establish the corresponding tractability results under suitable summability conditions on the general weights.

Tuesday June 9th – Morning/1, 11:30 – 12:00, JCMB Lecture Theatre C

Quasi-random Sampling in Diffusion Models

Session: Sampling and Machine Learning

p. 40

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Diffusion models are a leading framework for image and text generation. At a high level, they generate samples by transforming initial Gaussian noise through the time reversal of a stochastic differential equation. In this work, we study how quasi-random sampling of the initial Gaussian noise affects the resulting outputs. We find that antithetic sampling, pairing each noise realization with its negation, consistently produces strongly negatively correlated outputs in diffusion models. Remarkably, this phenomenon appears to be universal: it persists across datasets, model architectures, conditional and unconditional settings, and even beyond diffusion models to other generative frameworks. To explain this observation, we develop a theoretical perspective and propose a symmetry conjecture stating that the score function in the reverse diffusion dynamics is approximately affine-antisymmetric, a hypothesis supported by empirical evidence. This negative correlation yields substantial variance reduction for estimating certain metrics of the generative model. Building on this insight, we further extend the use of antithetic sampling to randomized quasi-Monte Carlo methods, and explore additional applications including improved sample diversity and image editing.

[1] Jing Jia, Sifan Liu, Bowen Song, Wei Yuan, Liyue Shen, Guanyang Wang. “Antithetic Noise in Diffusion Models.” International Conference on Learning Representations, 2026.

Tuesday June 9th – Morning/1, 11:30 – 12:00, JCMB 5326

Sequential Monte Carlo for Bayesian Inference Using Randomized Likelihoods

Session: Sampling and approximation for structured stochastic models in scientific computing, Part 1

p. 41

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In this talk we focus on Bayesian inverse problems in which the forward parameter-to-observable map is approximated in a stochastic way, for instance by Monte Carlo (MC) simulations. Such problems arise for example in uncertainty quantification of particle transport, where the parameter-to-observable map is defined through the solution of the Boltzmann equation. Approximating the likelihood with high accuracy requires MC simulations with many samples, which makes sampling from the posterior distribution expensive. We present an efficient method for sampling from the posterior based on pseudo-marginal sequential Monte Carlo (SMC) using likelihood tempering. To accelerate sampling from the posterior the method adopts a multilevel approach. A significant speedup is achieved compared to a single-level SMC using high-fidelity MC simulations while achieving the same error, which is demonstrated by numerical experiments.

Tuesday June 9th – Morning/1, 12:00 – 12:30, JCMB Lecture Theatre C

Flow-based Slice Sampling

Session: Sampling and Machine Learning

p. 40

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Slice sampling is a popular alternative to the classical Metropolis-Hastings (MH) algorithm for generating Markov chains to sample approximately from a given target distribution which is only known up to a normalizing constant. Slice sampling has some theoretical advantages over MH algorithms but on the other hand also the computational challenge to sample (approximately) from restrictions of the prior or reference measure to super-level sets of the likelihood. In this talk we study the use of flow matching, a state-of-the-art method in generative machine learning, for approximate sampling of these restricted measures, i.e., we learn a conditional generative flow. This is in contrast to the approach of transport (elliptical) slice sampling where a normalizing flow from posterior to a standard Gaussian reference measure is learned. We present the general ansatz, discuss some theoretical properties of the resulting flow-based slice sampling and show the performance as well as the limitations of the novel method in numerical experiments.

Tuesday June 9th – Morning/2, 10:30 – 11:00, JCMB 5327

On transport approaches to Bayesian optimal experimental design

Session: Optimal Experimental Design using Monte Carlo Methods

p. 42

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Bayesian optimal experimental design provides a principled framework for selecting informative data in inverse problems, but is often computationally challenging due to the need to sample from or approximate complex, high-dimensional probability distributions. This talk explores transport-based approaches for addressing these challenges. By constructing deterministic mappings between probability measures, transport methods enable efficient approximation of posterior and related quantities, facilitating the evaluation of design objectives. In particular, such mappings can be reused across multiple data realizations, enabling amortized inference in Bayesian settings. We discuss how such approaches can be used to improve the scalability of experimental design in Bayesian inverse problems and illustrate their potential in a range of settings.

Tuesday June 9th – Morning/2, 10:30 – 11:00, JCMB 5328

Tracking rare events within the ensemble Kalman filtering

Session: Advances in Monte Carlo methods for rare-event simulation, Part 1 p. 42

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In this work we employ importance sampling (IS) techniques to track a small over-threshold probability of a running maximum associated with the solution of a stochastic differential equation (SDE) within the framework of ensemble Kalman filtering (EnKF). Between two observation times of the EnKF, we propose to use IS with respect to the initial condition of the SDE, IS with respect to the Wiener process via a stochastic optimal control formulation, and combined IS with respect to both initial condition and Wiener process. Both IS strategies require the approximation of the solution of Kolmogorov Backward equation (KBE) with boundary conditions. Solving the KBE is computationally not feasible in high dimensions. To overcome this issue, we employ a Markovian projection dimension reduction technique to obtain an approximation of the solution of the KBE by just solving a one dimensional PDE. The proposed ideas are tested on two illustrative examples: Double Well SDE and Langevin dynamics, and showcase a significant variance reduction compared to the standard Monte Carlo method and another sampling-based IS technique, namely, multilevel cross entropy.

Tuesday June 9th – Morning/2, 10:30 – 11:00, JCMB 6206

Beta weighted bootstrap

Session: Statistical Approaches

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A standard Monte Carlo problem is to use bootstrap sampling to compute an asymptotic confidence interval for the mean of a random variable. The problem is very difficult in a nonparametric setting with small sample sizes. Most bootstrap intervals seriously undercover the target. The bootstrap t does comparably well but can produce very long

intervals with highly variable length, and is prone to infinitely long 95% intervals when used on discrete data. This talk presents a version of the weighted bootstrap t confidence intervals. The weights on the data points are drawn from a $\text{Beta}(1/2, 3/2)$ distribution. This gives second order accurate coverage, never gives infinite length intervals, and has a finite mean square bootstrap t statistic when there are at least three distinct sample values or two values that have appeared at least three times each. This work appears in arXiv:2508.10083.

Tuesday June 9th – Morning/2, 11:00 – 11:30, JCMB 5327

Sequential Bayesian design via Laplace policies

Session: Optimal Experimental Design using Monte Carlo Methods p. 42

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In recent years there has been significant development in policy-based approaches to sequential Bayesian experimental design. Here one aims to learn a mapping, called a policy, from the current knowledge state to the next design decision. Motivated by asymptotic theory, we introduce a policy-based approach that represents the knowledge state via the mean and variance of a Laplace approximation of the posterior. The performance of the new method is illustrated via examples. Additionally, we will describe how to conduct gradient based training, using the implicit function theorem and custom gradient methods to allow differentiable computation of the posterior modes. Our approach relies on “reparametrized” sampling to compute gradients, which does not apply directly to discrete random variables. Instead, we use concrete relaxation to adapt the methodology to the binary response case. Comparisons with other recent methods show that our method has superior performance in problems where the posterior is approximately Gaussian.

Tuesday June 9th – Morning/2, 11:00 – 11:30, JCMB 5328

Rare event estimation for multimodal and high-dimensional problems via subset adaptive importance sampling

Session: Advances in Monte Carlo methods for rare-event simulation, Part 1 p. 42

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Estimating rare events in complex systems is a key challenge in reliability analysis. The challenge grows in multimodal problems, where traditional methods often rely on a small set of design points and risk overlooking critical failure modes. Further, higher dimensions make the probability mass harder to capture and demand substantially larger sample sizes to estimate failures. In this talk, we propose a new sampling strategy, subset adaptive importance sampling (SAIS), that combines the strengths of subset simulation

and adaptive multiple importance sampling. SAIS iteratively refines a set of proposal distributions using weighted samples from previous stages, efficiently exploring complex and high-dimensional failure regions. Leveraging recent advances in adaptive importance sampling, SAIS yields low-variance estimates using fewer samples than state-of-the-art methods and achieves pronounced improvements in both accuracy and computational cost.

Tuesday June 9th – Morning/2, 11:00 – 11:30, JCMB 6206

Approximating evidence via bounded harmonic means

Session: Statistical Approaches

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Efficient Bayesian model selection relies on the model evidence or marginal likelihood, whose computation often requires evaluating an intractable integral. The harmonic mean estimator (HME) has long been a standard method of approximating the evidence. While computationally simple, the version introduced by Newton and Raftery (1994) potentially suffers from infinite variance. To overcome this issue, Gelfand and Dey (1994) defined a standardized representation of the estimator based on an instrumental function and Robert and Wraith (2009) later proposed to use higher posterior density (HPD) indicators as instrumental functions. Following this approach, a practical method is proposed, based on an elliptical covering of the HPD region with non-overlapping ellipsoids. The resulting estimator, called the Elliptical Covering Marginal Likelihood Estimator (ECMLE), not only eliminates the infinite-variance issue of the original HME and allows exact volume computations, but is also able to be used in multimodal settings. Through several examples, we illustrate that ECMLE outperforms other recent methods such as THAMES and its improved version (Metodiev et al 2024, 2025). Moreover, ECMLE demonstrates lower variance, a key challenge that subsequent HME variants have sought to address, and provides more stable evidence approximations, even in challenging settings.

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Tuesday June 9th – Morning/2, 11:30 – 12:00, JCMB 5327

Sparse Techniques for Regression in Deep Gaussian Processes

Session: Optimal Experimental Design using Monte Carlo Methods p. 42

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Gaussian processes (GPs) have gained popularity as flexible machine learning models for regression and function approximation with an in-built method for uncertainty quantification. However, GPs suffer when the amount of training data is large or when the underlying function contains multi-scale features that are difficult to represent by a stationary kernel. To address the former, training of GPs with large-scale data is often performed through inducing point approximations, also known as sparse GP regression (GPR), where the size of the covariance matrices in GPR is reduced considerably through a greedy search on the data set. To aid the latter, deep GPs have gained traction as hierarchical models that resolve multi-scale features by combining multiple GPs. Posterior inference in deep GPs requires a sampling or, more usual, a variational approximation. Variational approximations lead to large-scale stochastic, non-convex optimisation problems and the resulting approximation tends to represent uncertainty incorrectly. In this talk (and the associated preprint [1]), we combine variational learning with MCMC to develop a particle-based expectation-maximisation method to simultaneously find inducing points within the large-scale data (variationally) and accurately train the deep GPs (sampling-based). The result is a highly efficient and accurate methodology for deep GP training on large-scale data. We test our method on standard benchmark problems.

[1] Jonas Latz, Aretha L. Teckentrup, Simon Urbainczyk (2025): Sparse Techniques for Regression in Deep Gaussian Processes, arXiv:2505.11355.

Tuesday June 9th – Morning/2, 11:30 – 12:00, JCMB 5328

Importance sampling of unbounded random stopping times

Session: Advances in Monte Carlo methods for rare-event simulation, Part 1 p. 42

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Rare events in molecular dynamics are often related to noise-induced transitions between metastable states (protein folding, critical phase transitions, ...). The typical waiting times for such transitions are exponentially long compared to the characteristic timescale of the system, with no a priori upper bound. As a consequence, computing mean first exit times or committor probabilities by Monte Carlo requires to generate trajectories that can, in principle, become arbitrarily long. The long trajectories can cause problems for variance reduction methods like importance sampling that rely on the uniform integrability of likelihood ratios [1]. In this talk, we discuss rare event simulation by importance sampling based on convex transformations of the quantity of interest. The idea is to design importance sampling schemes that (a) reduce the variance of a

rare event estimator while controlling the average length of the trajectories and (b) that do not require to apply a change of measure to possibly very long trajectories [2]. We study different stochastic control formulations for committor and mean first exit times, which we compare both from a theoretical and a computational point of view, including numerical studies of some benchmark examples.

[1] Schütte, C., Klus, S., & Hartmann, C. (2023). Overcoming the timescale barrier in molecular dynamics: Transfer operators, variational principles and machine learning. *Acta Numerica*, 32, 517–673.

[2] Hartmann, C., Jöster, A., Schütte, C., Sikorski, A., & Weber, M. (2026). Importance sampling of unbounded random stopping times: computing committor functions and exit rates without reweighting. *arXiv preprint*, arXiv:2601.01489.

Tuesday June 9th – Morning/2, 11:30 – 12:00, JCMB 6206

Statistical Analysis of the Median as an Estimator of the Expectation Value

Session: Statistical Approaches

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Recent studies in randomized quasi-Monte Carlo research have generated considerable interest in using the empirical median instead of the empirical average to obtain a single estimate from r independently randomized point sets (ex. [1], [2]). The randomizations considered in these works yield favourable concentration inequalities for the individual estimates, which become even stronger for the empirical median via the “median trick”. However, there is a surprising lack of statistical analysis of the empirical median as an estimator in the finite-sample regime. In this talk, we use tools from convex analysis to characterize higher-moment conditions on the underlying sample distribution that are necessary for the empirical median to satisfy a prescribed bound on its expected error, and we derive lower bounds on the kurtosis required to achieve this level of performance. The resulting formula is explicit and applies to arbitrary error functions and any odd finite number of samples, providing a unified criterion for assessing whether a given error distribution permits median-based performance guarantees. In particular, this extends the discussion of [2] in exploring when the empirical median has smaller mean-square error than the empirical mean. We illustrate the relevance of the theory through applications to high-dimensional integration problems.

[1] T. Goda, K. Suzuki, M. Matsumoto. A universal median quasi-Monte Carlo integration. *SIAM J. Numer. Anal.* 62(1), 533–566 (2024).

[2] Z. Pan, A. Owen. Superpolynomial accuracy of multidimensional randomized nets using the median-of-means. *Math. Comp.* 93(349), 2265–2289 (2024).

Tuesday June 9th – Morning/2, 12:00 – 12:30, JCMB 5328

Rare event simulation via stochastic optimal control: new perspectives from diffusion-based sampling

Session: Advances in Monte Carlo methods for rare-event simulation, Part 1 p. 42

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Simulating rare events in stochastic environments requires carefully steering system dynamics toward regions of interest while maintaining unbiasedness through importance sampling in path space. This naturally leads to a formulation as a stochastic optimal control problem, where the objective is to minimize the variance of the associated Monte Carlo estimators.

Interestingly, closely related ideas have recently emerged in diffusion-based generative modeling. In these methods, a control function is learned to guide particles toward a prescribed target distribution. Such targets often exhibit isolated modes, which can be interpreted as rare events under the reference dynamics.

In this talk, I review both frameworks and highlight their theoretical connections, arguing that diffusion-based generative modeling can be viewed as a form of rare event forcing. Building on this perspective, I formulate the related stochastic optimal control problem as an optimization over path space measures and introduce a novel trust region approach tailored to rare event regimes. The resulting method provides explicit control over the variance of importance weights, yielding more stable and efficient algorithms for optimal control and sampling. Numerical experiments demonstrate the effectiveness of the approach for sampling highly multimodal distributions and for sampling rare transition paths in molecular dynamics.

Tuesday June 9th – Morning/2, 12:00 – 12:30, JCMB 6206

Constrained Matheron's update rule for truncated Gaussians with application to constrained Gaussian processes

Session: Statistical Approaches

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In this talk, we develop a new general method for sampling Gaussian vectors subject to linear equality and nonlinear inequality constraints. It is based on a modification of the Matheron's update rule (MUR) [1,4]. We provide theoretical results establishing its ability to accommodate large datasets and address high-dimensional linear regression problems. It is broadly applicable, as it accommodates both regression tasks and interpolation problems. The proposed method is robust and highly flexible. Its performance has been demonstrated in the context of Bayesian shape-restricted function estimation using both synthetic and real-world data. An efficient projection strategy is developed

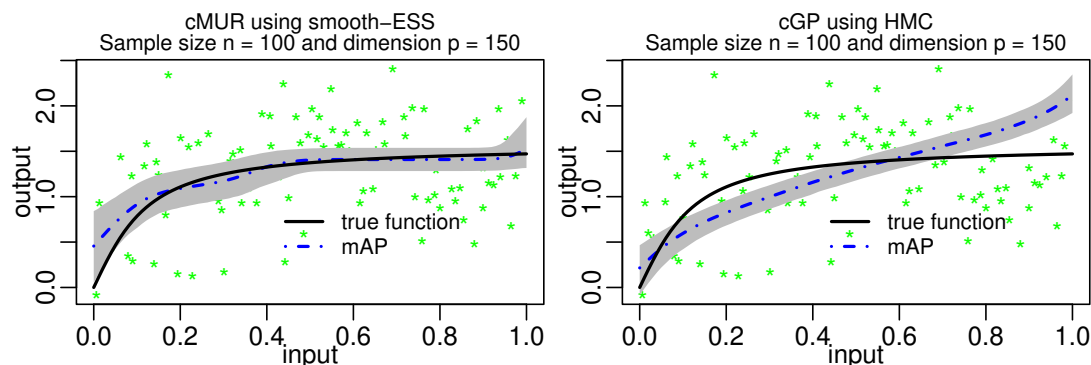


Figure 1: Monotone function estimation is performed using the finite-dimensional GP approximation of [2] with a joint truncated multivariate normal prior, employing two different sampling approaches: the proposed **cMUR** approach (left panel) and the *direct* Hamiltonian Monte Carlo (HMC) sampler [3] (right panel).

for sampling from an approximate posterior probability density function, ensuring that the posterior samples strictly satisfy the constraints.

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Tuesday June 9th – Afternoon/1, 15:30 – 16:00, JCMB Lecture Theatre A

Contractive kinetic Langevin samplers beyond global Lipschitz continuity

Session: *Stochastic computation and complexity, Part 3*

p. 43

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We examine the problem of sampling from log-concave distributions with (possibly) superlinear gradient growth under kinetic (underdamped) Langevin algorithms. Using

a carefully tailored taming scheme, we propose two novel discretizations of the kinetic Langevin SDE, and we show that they are both contractive and satisfy a log-Sobolev inequality. Building on this, we establish a series of non-asymptotic bounds in 2-Wasserstein and Total Variation distance between the law reached by each algorithm and the underlying target measure. This a joint work with Panagiotis Mertikopoulos.

Tuesday June 9th – Afternoon/1, 15:30 – 16:00, JCMB Lecture Theatre B

From optimisation to sampling: beyond gradient flows

Session: Mean Fields, Flows and Sampling

p. 43

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A common viewpoint in computational statistics is to cast sampling as the minimisation of a functional on the space of probability distributions, with the Bayesian posterior arising as a free-energy minimiser. Gradient-flow methods, including Wasserstein gradient flows, naturally lead to Langevin-type algorithms and connect sampling to optimisation. In this talk, I will discuss recent work that broadens this optimisation perspective beyond gradient flows, especially through saddle-point formulations and duality-gap techniques.

Tuesday June 9th – Afternoon/1, 15:30 – 16:00, JCMB Lecture Theatre C

Data-intrinsic approximation in metric spaces

Session: Sampling and approximation for structured stochastic models in scientific computing, Part 2

p. 44

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Analysis and processing of data is a vital part of our modern society and requires vast amounts of computational resources. To reduce the computational burden, compressing and approximating data has become a central topic. We consider the approximation of labeled data samples, mathematically described as site-to-value maps between finite metric spaces. Within this setting, we identify the discrete modulus of continuity as an effective data-intrinsic quantity to measure regularity of site-to-value maps without imposing further structural assumptions. We investigate the consistency of the discrete modulus of continuity in the infinite data limit and propose an algorithm for its efficient computation. Building on these results, we present a sample based approximation theory for labeled data. For data subject to statistical uncertainty we consider multilevel approximation spaces and a variant of the multilevel Monte Carlo method to compute statistical quantities of interest. Our considerations connect approximation theory for labeled data in metric spaces to the covering problem for (random) balls on the one hand and the efficient evaluation of the discrete modulus of continuity to combinatorial optimization on the other hand. We provide extensive numerical studies to illustrate the feasibility of the approach and to validate our theoretical results.

Tuesday June 9th – Afternoon/1, 15:30 – 16:00, JCMB 5326

Localized consensus-based sampling

Session: Interacting and Adaptive Particle Methods for Approximating Complex Distributions p. 45

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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 localized consensus-based method for sampling from non-Gaussian distributions. This method arises from an alternative derivation of consensus-based sampling (CBS). Starting from ensemble-preconditioned Langevin dynamics, we approximate the potential with a Moreau envelope, replace the gradient in the Langevin equation with a proximal operator, and finally approximate this operator by a weighted mean. Under Gaussian initial and target distributions, this procedure recovers the standard CBS dynamics, while retaining only the approximations valid beyond the Gaussian case yields a refined variant of polarized CBS [2]. The resulting algorithm, termed localized consensus-based sampling, is affine-invariant, converges exponentially for Gaussian targets in the mean-field limit, and demonstrates improved robustness over polarized CBS in numerical experiments.

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Tuesday June 9th – Afternoon/1, 16:00 – 16:30, JCMB Lecture Theatre A

Overcoming the temporal and spatial order barriers in approximating space-time white noise-driven SPDEs

Session: Stochastic computation and complexity, Part 3

p. 43

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We study the strong rate of convergence of fully discrete approximations of $1 + 1$ -dimensional space-time white noise-driven stochastic PDEs. A complete characterisation of the order of complexity is given in [Gyöngy '99] and [Davie - Gaines '01] in the multiplicative case, but the additive case remains largely open.

The best possible rate is conjectured to be much superior in the additive noise case, and [Jentzen - Kloeden '08] proposed a scheme that, in numerical experiments, does overcome the temporal order barrier that is present in the multiplicative case.

In our work, first, we prove the conjectured rate of the algorithm of [Jentzen - Kloeden '08], and second, we propose a new method that can also overcome the spatial order barrier.

Tuesday June 9th – Afternoon/1, 16:00 – 16:30, JCMB Lecture Theatre B

Non-convex entropic mean-field optimization via Best Response flow

Session: Mean Fields, Flows and Sampling p. 43

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We study the problem of minimizing non-convex functionals on the space of probability measures, regularized by the relative entropy (KL divergence) with respect to a fixed reference measure, as well as the corresponding problem of solving entropy-regularized non-convex-non-concave min-max problems. We utilize the Best Response flow (also known in the literature as the fictitious play flow) and study how its convergence is influenced by the relation between the degree of non-convexity of the functional under consideration, the regularization parameter and the tail behaviour of the reference measure. In particular, we demonstrate how to choose the regularizer, given the non-convex functional, so that the Best Response operator becomes a contraction with respect to the L^1 -Wasserstein distance, which ensures the existence of its unique fixed point that is then shown to be the unique global minimizer for our optimization problem. This extends recent results where the Best Response flow was applied to solve convex optimization problems regularized by the relative entropy with respect to arbitrary reference measures, and with arbitrary values of the regularization parameter. Our results explain precisely how the assumption of convexity can be relaxed, at the expense of making a specific choice of the regularizer. Additionally, we demonstrate how these results can be applied in reinforcement learning in the context of policy optimization for Markov Decision Processes and Markov games with softmax parametrized policies in the mean-field regime.

Tuesday June 9th – Afternoon/1, 16:00 – 16:30, JCMB Lecture Theatre C

Free Energy Barriers in Bayesian Logistic Regression

Session: Sampling and approximation for structured stochastic models in scientific computing, Part 2 p. 44

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Bayesian methods have become increasingly popular as they provide a direct way to quantify uncertainty. However to take advantage of this one must be able to sample the posterior. To sample general posteriors one is reliant on MCMC methods. It was shown in the paper by Bandeira and coauthor in 2022 the existence of a free energy barrier in the high dimensional setting can cause computation difficulties for local MCMC methods. In this talk we will give an introduction to free energy barriers and show numerical results for the high dimensional Bayesian logistic regression.

Tuesday June 9th – Afternoon/1, 16:00 – 16:30, JCMB 5326

Greedy Mixture Approximation: A Unified Algorithmic Framework

Session: Interacting and Adaptive Particle Methods for Approximating Complex Distributions p. 45

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A vast range of methods aim to approximate a probability distribution by a computationally tractable representation. Among these, an important class consists of algorithms constructing or calibrating a mixture distribution, i.e. a weighted sum of simple components such as Gaussian or Student's t-distributions.

This talk presents a unifying framework for a class of greedy mixture methods which, starting from an initial approximation, iteratively add new components and progressively improve the approximation. We show that a range of seemingly distinct approaches—including iterated Laplace approximation, incremental and adaptive multiple importance sampling (IMIS/AMIS), variational boosting, and kernel-based methods such as kernel herding—can all be understood within the framework. We formulate general convergence results for the unified framework, and show that they apply to existing methods under suitable assumptions. Finally, we provide systematic numerical benchmarking across various targets and performance metrics, with particular emphasis on importance sampling, where mixture approximations naturally yield efficient proposal distributions.

Tuesday June 9th – Afternoon/1, 16:30 – 17:00, JCMB Lecture Theatre A

A Control Variate Method Driven by Diffusion Approximation

Session: Stochastic computation and complexity, Part 3 p. 43

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We present a control variate estimator for a quantity that can be expressed as the expectation of a functional of a random process, that is itself the solution of a differential equation driven by fast mean-reverting ergodic forces. The control variate is the expectation of the same functional for the limit diffusion process that approximates the

original process when the mean-reversion time goes to zero. To get an efficient control variate estimator, we propose a coupling method to build the original process and the limit diffusion process. We show that the correlation between the two processes indeed goes to one when the mean reversion time goes to zero and we quantify the convergence rate, which makes it possible to characterize the variance reduction of the proposed control variate method. The efficiency of the method is illustrated on a few examples. This is joint work with Josselin Garnier (École Polytechnique, France). Link to the paper: <https://doi.org/10.1002/cpa.21976>

Tuesday June 9th – Afternoon/1, 16:30 – 17:00, JCMB Lecture Theatre B

Data-driven approximation of transfer operators for mean-field stochastic differential equations

Session: Mean Fields, Flows and Sampling

p. 43

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Mean-field stochastic differential equations, also called McKean–Vlasov equations, are the limiting equations of interacting particle systems with fully symmetric interaction potential. Such systems play an important role in a variety of fields ranging from biology and physics to sociology and economics. Global information about the behavior of complex dynamical systems can be obtained by analyzing the eigenvalues and eigenfunctions of associated transfer operators such as the Perron–Frobenius operator and the Koopman operator. In this paper, we extend transfer operator theory to McKean–Vlasov equations and show how extended dynamic mode decomposition and the Galerkin projection methodology can be used to compute finite-dimensional approximations of these operators, which allows us to compute spectral properties and thus to identify slowly evolving spatiotemporal patterns or to detect metastable sets. The results will be illustrated with the aid of several guiding examples and benchmark problems including the Cormier model, the Kuramoto model, and a three-dimensional generalization of the Kuramoto model.

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

[1] Ioannou, E., Klus, S. and dos Reis, G., 2025. Data-driven approximation of transfer operators for mean-field stochastic differential equations. arXiv preprint arXiv:2509.09891.

Tuesday June 9th – Afternoon/1, 16:30 – 17:00, JCMB Lecture Theatre C

Efficient sampling of deep Gaussian processes via wavelet sparsity

Session: Sampling and approximation for structured stochastic models in scientific computing, Part 2

p. 44

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Deep Gaussian processes provide a flexible framework for modelling complex, non-stationary random fields, but sampling from these models is typically computationally expensive.

In this talk, we present a wavelet-based approach to sampling from deep Gaussian processes. By representing the associated covariance operators in a multiresolution wavelet basis, we obtain sparse approximations that reduce the cost of sampling from cubic to near-linear complexity.

We establish error estimates for the resulting approximations and analyse how these propagate through the layers of the deep Gaussian process. Numerical experiments demonstrate that the method achieves substantial computational savings while maintaining accuracy.

Tuesday June 9th – Afternoon/1, 16:30 – 17:00, JCMB 5326

Importance Reweighting of Interacting Particle Samplers

Session: Interacting and Adaptive Particle Methods for Approximating Complex Distributions p. 45

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Interacting particle samplers generate sequences of particle ensembles on the way to a target distribution, yet in practice almost all intermediate particles are discarded and only the final ensemble is used. Moreover, these particles typically do not follow the target distribution exactly, as they arise from approximate interacting dynamics.

This talk presents an alternative approach that recycles the full particle history. The Gaussian update laws underlying methods such as ALDI and EKS are interpreted as proposal distributions for importance sampling. By reweighting particles across ensemble members and time steps, one obtains consistent estimators that exploit all generated particles. Several importance-reweighting strategies based on individual and mixture proposals are discussed, together with their advantages when target evaluations are computationally expensive.

Tuesday June 9th – Afternoon/1, 17:00 – 17:30, JCMB Lecture Theatre A

Weak approximation of kinetic SDEs: closing the criticality gap

Session: Stochastic computation and complexity, Part 3 p. 43

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We study the weak convergence of a generic tamed Euler-Maruyama scheme for kinetic stochastic differential equations (SDEs) with integrable drifts. We show that the marginal density of the considered scheme converges at rate $1/2$ to the corresponding marginal

density of the SDE. The convergence rate is independent from the criticality gap, which is new compared to previous results.

Tuesday June 9th – Afternoon/1, 17:00 – 17:30, JCMB Lecture Theatre B

A Computable Measure of Suboptimality for Entropy-Regularised Variational Objectives

Session: Mean Fields, Flows and Sampling

p. 43

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Several emerging post-Bayesian methods target a probability distribution for which an entropy-regularised variational objective is minimised. This increased flexibility introduces a computational challenge, as one loses access to an explicit unnormalised density for the target. To mitigate this difficulty, we introduce a novel measure of suboptimality called ‘gradient discrepancy’, and in particular a ‘kernel’ gradient discrepancy (KGD) that can be explicitly computed. In the standard Bayesian context, KGD coincides with the kernel Stein discrepancy (KSD), and we obtain a novel characterisation of KSD as measuring the size of a variational gradient. Outside this familiar setting, KGD enables novel sampling algorithms to be developed and compared, even when unnormalised densities cannot be obtained. To illustrate this point several novel algorithms are proposed and studied, including a natural generalisation of Stein variational gradient descent, with applications to mean-field neural networks and predictively oriented posteriors presented. On the theoretical side, our principal contribution is to establish sufficient conditions for desirable properties of KGD, such as continuity and convergence control.

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

[1] Chazal C, Kanagawa H, Shen Z, Korba A, Oates CJ (2025) A Computable Measure of Suboptimality for Entropy-Regularised Variational Objectives. [arXiv:2509.10393](https://arxiv.org/abs/2509.10393).

Tuesday June 9th – Afternoon/2, 15:30 – 16:00, JCMB 5327

Dimension-independent convergence rates of median randomized nets

Session: Frontiers in QMC methods, Part 2

p. 45

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Recent advances in quasi-Monte Carlo integration demonstrate that the median of linearly scrambled digital net estimators achieves near-optimal convergence rates for high-dimensional integrals without requiring a priori knowledge of the integrand’s smoothness. Building on this framework, we prove that the median estimator attains dimension-independent convergence, a property known as strong tractability in complexity theory, under tractability conditions characterized by low effective dimensionality. Using a

probabilistic, integrand-specific error criterion, our analysis establishes both faster and dimension-independent convergence under weaker assumptions than previously possible in the worst-case setting.

Tuesday June 9th – Afternoon/2, 15:30 – 16:00, JCMB 5328

Estimating rare-event probabilities associated with the McKean–Vlasov equation

Session: Advances in Monte Carlo methods for rare-event simulation, Part 2 p. 46

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This talk addresses the efficient Monte Carlo estimation of rare-event probabilities associated with a broad class of McKean–Vlasov stochastic differential equations (MV-SDEs), which arise in the analysis of mean-field systems in statistical physics, mathematical finance, and collective behaviour models. Standard Monte Carlo methods become computationally infeasible in this setting due to the rapid growth of the estimator’s relative variance (coefficient of variation) in the rare-event regime. Using stochastic optimal control, an optimal importance sampling measure change is constructed to minimise the variance of the resulting estimator. The resulting double-loop Monte Carlo (DLMC) estimator with importance sampling significantly mitigates this growth in the coefficient of variation. The framework is further extended to the multilevel and multi-index Monte Carlo settings to reduce computational complexity, leveraging propagation-of-chaos results to ensure that the level and mixed-differences vanish in the mean-field limit. To address the discontinuity of the probability observable, both analytical and numerical smoothing techniques are introduced to recover optimal variance convergence rates. As a result, the computational complexity required to achieve relative accuracy TOL_r is reduced from $\mathcal{O}(\text{TOL}_r^{-5})$ for a single-cloud importance sampling estimator to $\mathcal{O}(\text{TOL}_r^{-4})$ for DLMC, $\mathcal{O}(\text{TOL}_r^{-3})$ for multilevel DLMC, and $\mathcal{O}(\text{TOL}_r^{-2} (\log \text{TOL}_r)^2)$ for multi-index DLMC. Numerical experiments on linear mean-field, Kuramoto, and Cucker–Smale models demonstrate computational savings of several orders of magnitude compared with standard Monte Carlo.

Tuesday June 9th – Afternoon/2, 15:30 – 16:00, JCMB 6206

Knots and variance ordering of sequential Monte Carlo algorithms

Session: Sequential Monte Carlo and Importance Sampling

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Sequential Monte Carlo algorithms, or particle filters, are widely used for approximating intractable integrals, particularly those arising in Bayesian inference and state-space

models. We introduce a new variance reduction technique, the knot operator, which improves the efficiency of particle filters by incorporating potential function information into part, or all, of a transition kernel. The knot operator induces a partial ordering of Feynman–Kac models that implies an order on the asymptotic variance of particle filters, offering a new approach to algorithm design. We discuss connections to existing strategies for designing efficient particle filters, including model marginalisation. Our theory generalises such techniques and provides quantitative asymptotic variance ordering results. We revisit the fully-adapted (auxiliary) particle filter using our theory of knots to show how a small modification guarantees an asymptotic variance ordering for all relevant test functions.

Preprint: <https://arxiv.org/abs/2510.01901>.

Tuesday June 9th – Afternoon/2, 16:00 – 16:30, JCMB 5327

Coarse scrambling for Sobol’ and Niederreiter sequences

Session: Frontiers in QMC methods, Part 2

p. 45

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We introduce *coarse scrambling*, a novel randomization for digital sequences that permutes blocks of digits in a mixed-radix representation. This construction is designed to preserve the $(0, \mathbf{e}, d)$ -sequence property of the underlying points. For sufficiently smooth integrands, we prove that this method achieves the canonical $O(n^{-3+\epsilon})$ variance decay rate, matching that of standard Owen’s scrambling. Crucially, we show that its maximal gain coefficient grows only logarithmically with dimension, $O(\log d)$, thus providing theoretical robustness against the curse of dimensionality affecting scrambled Sobol’ sequences.

Tuesday June 9th – Afternoon/2, 16:00 – 16:30, JCMB 5328

Hierarchical Importance Sampling for Estimating Occupation Times of SDE Solutions

Session: Advances in Monte Carlo methods for rare-event simulation, Part 2

p. 46

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This study addresses the estimation of the complementary cumulative distribution function of the occupation time for a process governed by a stochastic differential equation. We focus on rare events in the right tail, where variance reduction is crucial for computational efficiency. Building on the connection between importance sampling (IS) and stochastic optimal control, we propose an optimal single-level IS (SLIS) estimator based on the solution of an auxiliary Hamilton–Jacobi–Bellman partial differential equation. The cost of solving this equation is included in the total computational work, and

an optimal balance between preprocessing and sampling is derived. The approach is extended to a multilevel IS (MLIS) estimator, for which the single-level variance vanishes as the discretization level increases due to the zero-variance property of the optimal control. This leads to a necessary and sufficient condition under which MLIS outperforms SLIS. To ensure this condition, we introduce a smoothing of the drift and observable, together with a common-likelihood MLIS formulation that preserves variance decay. Numerical experiments on fade duration estimation confirm the theoretical results and demonstrate substantial efficiency gains over SLIS.

1. Stochastic differential equations for performance analysis of wireless communication systems. Published in IEEE Transactions on Wireless Communications (Ben Amar, Ben Rached, Raul Tempone, et al. 2025).
2. Hierarchical Importance Sampling for Estimating Occupation Time in SDE Solutions. Submitted to arXiv (Ben Amar, Ben Rached, and Raul Tempone 2025).

Tuesday June 9th – Afternoon/2, 16:00 – 16:30, JCMB 6206

Collective Annealing by Switching Temperatures: a Boltzmann-type framework

Session: Sequential Monte Carlo and Importance Sampling

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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. Importantly, one is free to sample from any scaled normal-like distribution. 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.

We wish to improve a few key components of these algorithms. First, three popular cooling schedules in the literature are inverse logarithmic in time (Classical Simulated Annealing), inverse in time (Fast Simulated Annealing) and a generalization of the two (Generalized Simulated Annealing). However, we will 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. Second,

classic Metropolis-Hastings is usually not suited for badly scaled problems. Furthermore, the acceptance probability can sometimes freeze particles in local minima too early in the simulation due to overly hasty cooling or steep hills. We will therefore use an adapted Metropolis-Hastings strategy to overcome these issues.

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, Griewank, Schwefel, Rosenbrock, etc.) that this novel approach outperforms popular SA algorithms.

Tuesday June 9th – Afternoon/2, 16:30 – 17:00, JCMB 5327

A median QMC method for unbounded integrands over \mathbb{R}^s in weighted unanchored Sobolev spaces

Session: Frontiers in QMC methods, Part 2

p. 45

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This talk focuses on quasi-Monte Carlo (QMC) integration of Lebesgue integrable functions with respect to a density function over \mathbb{R}^s . We extend the construction-free median QMC rule proposed by Goda and L'ecuyer (SIAM J. Sci. Comput., 2022) to the weighted unanchored Sobolev space of functions defined over \mathbb{R}^s introduced by Nichols and Kuo (J. Complexity, 2014). By taking the median of $k = \mathcal{O}(\log N)$ independent randomized QMC estimators, we prove that for any $\epsilon \in (0, r - \frac{1}{2}]$, our method achieves a mean absolute error bound of $\mathcal{O}(N^{-r+\epsilon})$, where N is the number of points and $r > \frac{1}{2}$ is a parameter determined by the function space. This rate matches the rate of randomly shifted lattice rules obtained via a component-by-component (CBC) construction, while our approach requires no specific CBC constructions or prior knowledge of the space's weight structure. Numerical experiments demonstrate that our method attains an accuracy comparable to the CBC construction based method, and outperforms the Monte Carlo method.

Tuesday June 9th – Afternoon/2, 16:30 – 17:00, JCMB 5328

Variance Reduction with Importance Sampling for Optimization Under Rare Chance Constraints

Session: Advances in Monte Carlo methods for rare-event simulation, Part 2

p. 46

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Chance constraints emerge naturally in the context of enhancing the resilience of engineering systems, particularly those exposed to high-impact but rare events such as natural disasters, infrastructure failures, supply disruptions, and financial crashes. However, the

rarity of such events renders solving chance-constrained models using direct sample average approximation methods highly impractical. Importance sampling can be a viable solution method in such cases, as it employs an alternative probability distribution to generate samples more frequently from the rare-event regions. The key challenge, however, lies in informing how to select alternative distributions that remain effective across the decision space and in diverse problem settings. Our work employs self-structuring importance samplers to develop a new sampling-based solution procedure for a broad class of chance-constrained optimization problems. The algorithm transforms samples generated through direct Monte Carlo into importance samples which accurately represent the rare region behavior and can be applied uniformly alike across a wide range of constraint functions and probability distributions. Our results demonstrate that the proposed algorithm offers asymptotically optimal variance reduction and can substantially outperform Monte Carlo sampling in terms of both feasibility and optimality, even with small sample sizes.

Tuesday June 9th – Afternoon/2, 16:30 – 17:00, JCMB 6206

Spectral gap in parallel tempering: a variational analysis

Session: Sequential Monte Carlo and Importance Sampling

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Parallel tempering is a popular MCMC-based method for sampling from Gibbs measures, designed to avoid the pitfall of getting trapped in potential wells in the low-temperature regime. Previous mathematical work on the convergence of parallel tempering has focused on particular classes of potential functions, or to the extent that more general potentials are considered, the results are asymptotic or deal with convergence senses which are weaker than in total variation. In this talk, we present a spectral gap bound for parallel tempering which holds for general potential functions, in both discrete and diffusive settings. The bound provides insight into practical matters of implementation, confirming the near optimality of a geometric sequence of temperatures and also shedding light on the optimal number of chains at which to run the algorithm and the influence of dimension. The bound depends on the internal energy of the Gibbs ensemble, and when the temperatures are chosen near optimally, one obtains a relaxation time which is polynomial in the inverse lowest temperature. The proof of this result works directly with the variational characterization of the spectral gap and exploits the structure of the Dirichlet form associated with the parallel tempering process.

Tuesday June 9th – Afternoon/2, 17:00 – 17:30, JCMB 5327

Fourier Neural Operators on Rank-1 Lattices

Session: Frontiers in QMC methods, Part 2

p. 45

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The Fourier Neural Operator (FNO) [1] is a neural network architecture that learns mappings between function spaces. Its efficient implementation is based on the multi-dimensional Fourier transform. We prove that the generalization error of the FNO can be improved by replacing Cartesian tensor product grids by carefully constructed quasi-Monte Carlo point sets. Using rank-1 lattices, we achieve more accurate and efficient approximations from fewer parameters and training samples. In addition, the architecture is simplified, because the high-dimensional Fourier transform on rank-1 lattices requires only a one-dimensional fast Fourier transform. We demonstrate the benefits of FNOs on rank-1 lattices for the example of a parametric partial differential equation (PDE).

- [1] 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.

Tuesday June 9th – Afternoon/2, 17:00 – 17:30, JCMB 6206

On the interpretation of diagnostics in importance sampling: α -ESS and tail indices

Session: Sequential Monte Carlo and Importance Sampling

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Importance sampling is a popular Monte Carlo methodology to approximate integrals with respect to an intractable target density. Instead of sampling directly from this intractable density, importance sampling uses samples from a well-chosen proposal density and reweights these samples accordingly. Importance sampling has been widely used in Bayesian statistics, rare-event estimation, and as a key component of sequential Monte Carlo methods. However, assessing the quality of the proposal is a difficult task and various diagnostics have been proposed. The most widely used diagnostic is the effective sample size (ESS), which is easy to compute and interpret but amounts to diagnose importance sampling performance by computing another importance sampling estimator with the same proposal. Generalized versions of the ESS, called α -ESS, have thus been proposed and shown to be more robust in practice [5, 3, 1, 2, 4]. Alternatively, a diagnostic based on tail indices have also been proposed [6]. In this work, we investigate the conclusions one can draw from using these diagnostics. We explain the empirical performance of α -ESS and show that they can be used to detect some poorly-designed proposals but can also lead to erroneous conclusions on the choice of the proposal density. We also show that α -ESS and tail indices are mostly independent. These theoretical developments are backed by numerical experiments and allow to derive some guidelines for practitioners.

[1] S. Chatterjee and P. Diaconis. The sample size required in importance sampling. *The Annals of Applied Probability*, 28(2):1099–1035, 2018.

[2] V. Elvira, L. Martino, and C. P. Robert. Rethinking the effective sample size. *International Statistical Review*, 99(3):525–550, 2022.

[3] J. H. Huggins and D. M. Roy. Sequential Monte Carlo as approximate sampling: Bounds, adaptive resampling via ∞ -ESS, and an application to particle Gibbs. *Bernoulli*, 25(1):584–622, 2019.

[4] L. Martino and V. Elvira. Effective sample size approximations and entropy measures. *Computational Statistics*, 40:5433–5464, 2025.

[5] L. Martino, V. Elvira, and F. Louzada. Effective sample size for importance sampling based on discrepancy measures. *Signal Processing*, 131:386–401, 2017.

[6] A. Vehtari, D. Simpson, A. Gelman, Y. Yao, and J. Gabry. Pareto smoothed importance sampling. *Journal of Machine Learning Research*, 25(72):1–58, 2024.

Wednesday June 10th – 1, 10:30 – 11:00, JCMB Lecture Theatre A

Flatness-Aware Stochastic Gradient and Zeroth-Order Langevin Dynamics

Session: Stochastic computation and complexity, Part 4

p. 47

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Flatness of the loss landscape plays a central role in understanding the dynamics and generalization behavior of modern learning algorithms. Motivated by this perspective, we introduce Flatness-Aware Stochastic Gradient Langevin Dynamics (fSGLD), a first-order stochastic optimization method that biases its dynamics toward flatter regions while preserving the computational and memory efficiency of SGD and SGLD. We provide a non-asymptotic analysis showing that fSGLD converges to a flatness-biased Gibbs distribution under a theoretically prescribed coupling between the noise scale σ and the inverse temperature β , together with explicit excess risk guarantees. Empirical evaluations on standard optimizer benchmarks, Bayesian image classification, uncertainty quantification, and out-of-distribution detection demonstrate consistently strong performance and reliable uncertainty calibration. Time permitting, we will also discuss a zeroth-order extension of fSGLD that enables flatness-aware stochastic sampling in gradient-free settings.

References:

[1] Stefano Bruno, Youngsik Hwang, Jaehyeon An, Sotirios Sabanis, Dong-Young Lim, Flatness-Aware Stochastic Gradient Langevin Dynamics, Arxiv, 2025.

[2] Stefano Bruno & Dong-Young Lim, Zeroth-Order Langevin Dynamics for Non-convex Optimization: Global Convergence to Curvature-Regularized Minima, To appear.

Wednesday June 10th – 1, 10:30 – 11:00, JCMB Lecture Theatre B

A multimodal Laplace approximation

Session: Approximation and sampling of concentrated posterior distributions

p. 47

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In Bayesian learning, sampling from the posterior distribution is generally a challenging task, especially when the posterior is not strongly log-concave. For instance, as the posterior distribution concentrates with an increasing number of observations, classical MCMC methods may fail to adequately explore the entire parameter space. In this presentation, I introduce a multimodal extension of the Laplace approximation and derive bounds on the Hellinger distance between this approximation and the true posterior distribution. This approximation will be exploited to design new sampling methods for posterior distributions.

Wednesday June 10th – 1, 10:30 – 11:00, JCMB Lecture Theatre C

Diffusion Annealed Langevin Monte Carlo for Generative Modelling and Sampling

Session: Gradient Flows and Continuous-time Markov Processes in Data Science and Beyond p. 48

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Coauthor(s): Matthew Young, Sebastian Reich, Andrew Duncan, Deniz Akyildiz

In this talk, we study the theoretical properties of general diffusion paths and their Langevin Monte Carlo implementation, termed diffusion annealed Langevin Monte Carlo (DALMC), under weak assumptions on the data distribution. We derive non-asymptotic error bounds for annealed Langevin dynamics where the path of distributions is given by Gaussian convolutions of the data, as in diffusion models. We then extend the analysis to heavy-tailed (Student's t) diffusion paths, establishing — for the first time — their theoretical validity for heavy-tailed data. These results provide rigorous guarantees for a class of score-based generative models that interpolate between a simple distribution (Gaussian or Student's t) and the data in finite time, offering a broader perspective than standard diffusion approaches based on a forward Ornstein–Uhlenbeck process.

Building on this framework, we introduce new methods for efficient sampling from complex, unnormalised targets via diffusion paths. We present different challenges when using diffusion paths and provide different algorithms to overcome them.

Wednesday June 10th – 1, 10:30 – 11:00, JCMB 5326

Single- and Multi-Level Fourier-RQMC Methods for Multivariate Shortfall Risk

Session: Recent advances in hierarchical methods for uncertainty quantification, Part 1 p. 49

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Multivariate shortfall risk measures provide a principled framework for quantifying systemic risk and determining capital allocations prior to aggregation in interconnected

financial systems. Despite their well-established theoretical properties, the numerical estimation of multivariate shortfall risk and the corresponding optimal allocations remains computationally challenging, as existing Monte Carlo based approaches can be numerically expensive due to slow convergence.

In [1], we develop a new class of single and multilevel numerical algorithms for estimating multivariate shortfall risk and the associated optimal allocations, based on a combination of Fourier inversion techniques and randomized quasi-Monte Carlo (RQMC) sampling. Rather than operating in physical space, our approach evaluates the relevant expectations appearing in the risk constraint and its optimization in the frequency domain, where the integrands exhibit enhanced smoothness properties that are well suited for RQMC integration. We establish a rigorous mathematical framework for the resulting Fourier RQMC estimators, including convergence analysis and computational complexity bounds. Beyond the single level method, we introduce a multilevel RQMC scheme that exploits the geometric convergence of the underlying deterministic optimization algorithm to reduce computational cost while preserving accuracy. Numerical experiments demonstrate that the proposed Fourier RQMC methods outperform sample average approximation and stochastic optimization benchmarks in terms of accuracy and computational cost across a range of models for the risk factors and loss structures. Consistent with the theoretical analysis, these results demonstrate improved asymptotic convergence and complexity rates relative to the benchmark methods, with additional savings achieved through the proposed multilevel RQMC construction.

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Wednesday June 10th – 1, 11:00 – 11:30, JCMB Lecture Theatre A

Exact asymptotic error and optimality of adaptive Milstein scheme for global approximation of SDEs with countably dimensional noise

Session: Stochastic computation and complexity, Part 4

p. 47

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In this talk, we study global approximation of solutions to the following stochastic differential equation

$$\begin{cases} dX(t) = a(t, X(t)) dt + b(t, X(t)) dW(t), & t \in [0, T], \\ X(0) = x_0 \in \mathbb{R}, \end{cases} \quad (1)$$

where $T > 0$, $W(t) = [W_1(t), W_2(t), \dots]^T$ is a countable sequence of independent scalar Wiener processes, thus extending the setting of [2]. Under suitable regularity conditions and the noise commutativity property imposed on the model coefficients, we construct a truncated-dimension Milstein scheme with path-independent step-size control and derive an explicit formula for its asymptotic error. The corresponding asymptotic terms depend only on the diffusion via its Hilbert-Schmidt norm:

$$\int_0^T \left(\mathbb{E} \|b(t, X(t))\|_{HS}^2 \right)^{1/2} dt.$$

We also analyse approximation errors within the class of methods $\bar{X} = (\bar{X}_{M_n, k_n})_{n=1}^\infty$ that are indexed by the discretisation parameter k_n and Wiener process truncation levels M_n . Therein, the cost of an admissible scheme is defined as the number of scalar evaluations of the Wiener process. We prove that the constructed Milstein scheme asymptotically attains the minimal error bound among all (possibly adaptive) methods using the same truncation sequence $(M_n)_{n=1}^\infty$, and is therefore optimal.

Suitable variations of the main result are presented for the subclass of methods utilising equidistant (non-adaptive) meshes, and for SDEs driven by a finite-dimensional Wiener process.

[1] Ł. Ste piń, Exact asymptotic error and optimality of adaptive Milstein scheme for global approximation of SDEs with countably dimensional noise, in preparation, 2026+

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[3] P. Przybyłowicz, M. Sobieraj, Ł. Ste piń, Efficient approximation of SDEs driven by countably dimensional Wiener process and Poisson random measure, *SIAM J. Numer. Anal.* **60** (2022), 824–855.

Wednesday June 10th – 1, 11:00 – 11:30, JCMB Lecture Theatre B

Multimodal Laplace-based sampling

Session: Approximation and sampling of concentrated posterior distributions p. 47

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Building on the approximation result in Hellinger distance, we study the use of a multimodal Laplace approximation as a proposal distribution for both importance sampling and the independent Metropolis–Hastings algorithm, and analyze the efficiency of these methods for targeting concentrating multimodal posteriors. For importance sampling, we quantify efficiency via the effective sample size and establish convergence rates in the regime of increasingly concentrated posterior distributions. For the independent Metropolis–Hastings algorithm, we derive convergence rates for the average acceptance probability, the lag-one autocorrelation, and the spectral gap. Finally, we validate our theoretical findings through numerical experiments.

Wednesday June 10th – 1, 11:00 – 11:30, JCMB Lecture Theatre C

An optimal experimental design approach to sensor placement in continuous stochastic filtering

Session: Gradient Flows and Continuous-time Markov Processes in Data Science and Beyond p. 48

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Sequential filtering and spatial inverse problems assimilate data points distributed either temporally (in the case of filtering) or spatially (in the case of spatial inverse problems). Sometimes it is possible to choose the position of these data points (which we call sensors here) in advance, with the goal of maximising the expected information gain (or a different metric of performance) from future data, and this leads to an Optimal Experimental Design (OED) problem. Here we revisit an interpretation of optimising sensor placement as an integration with respect to a general probability measure ξ . This generalises the problem of discrete-time sensor placement (which corresponds to the special case where the probability measure is a mixture of Diracs) to an infinite-dimensional, but mathematically more well-behaved setting. We focus on the continuous-time stochastic filtering setting, whose solution is governed by the Zakai equation. We derive an expression for the Fréchet derivative of a general OED utility functional, the key to which is an adjoint (backwards in time) differential equation. This paves the way for utilising new gradient-based methods for solving the corresponding optimisation problem, as a potentially more efficient alternative to (semi-)discrete optimisation methods, e.g. based on greedy insertion and deletion of sensor placements

This talk is about recent results in “An optimal experimental design approach to sensor placement in continuous stochastic filtering.” *Statistics and Computing* 36.3 (2026): 102.

Wednesday June 10th – 1, 11:00 – 11:30, JCMB 5326

Hierarchical Delayed Acceptance using Gaussian Process Surrogates

Session: Recent advances in hierarchical methods for uncertainty quantification, Part 1
p. 49

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Solving Bayesian inverse problems for expensive computational models can be made more feasible by using hierarchical methods and surrogates. With this goal, we explore Multilevel Delayed Acceptance-type (MLDA) algorithms, as introduced by Lykkegaard et al., 2023, in application to a linear elasticity toy problem, which is an easily controllable well-posed setting. We explore model hierarchies of Finite Element-based solvers and Gaussian process emulators (GPE), with the aim to better understand the viability of different setups in the hierarchical sampling algorithms that include GPE as cheap model approximations on the lower levels of the hierarchy. The findings can be taken as indicative for the viability of MLDA for truly complex and expensive computational models, which find application in e.g. material sciences, geophysics and computational astrophysics.

[1] Cui et al. (2011), *Bayesian calibration of a large-scale geothermal reservoir model by a new adaptive delayed acceptance Metropolis Hastings algorithm*, Water Resources Research, vol. 47, issue 10.

[2] Cui et al. (2019), *A posteriori stochastic correction of reduced models in delayed-acceptance MCMC, with application to multiphase subsurface inverse problems*, International Journal for Numerical Methods in Engineering, vol. 118, pp. 578–605.

[3] Lykkegaard et al. (2023), *Multilevel Delayed Acceptance MCMC*, SIAM/ASA Journal on Uncertainty Quantification, vol. 11, pp. 1–30.

Wednesday June 10th – 1, 11:30 – 12:00, JCMB Lecture Theatre A

On lower error bounds for strong approximation of SDEs with Hölder continuous drift coefficient

Session: Stochastic computation and complexity, Part 4

p. 47

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

$$\begin{aligned} dX_t &= \mu(X_t) dt + dW_t, \quad t \in [0, 1], \\ X_0 &= x_0 \end{aligned} \tag{2}$$

at the final time point 1 in the case that the drift coefficient μ is bounded and 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 show that for such SDEs, an L^p -error rate better than $(1+\alpha)/2$ can not be achieved in general by no numerical method based on finitely many evaluations of W and its integrals at fixed time points. In particular, Wagner–Platen type schemes are not superior to the Euler scheme with respect to the L^p -error rate in this setting in general. 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].

This is the first lower bound in the literature for the L^p -approximation of the solution of an SDE at the final time point by numerical methods based on finitely many evaluations of W and its integrals.

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Wednesday June 10th – 1, 11:30 – 12:00, JCMB Lecture Theatre B

High-dimensional Laplace asymptotics up to the concentration threshold

Session: Approximation and sampling of concentrated posterior distributions p. 47

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Concentrated, high-dimensional posterior distributions can be expressed in the form

$$\pi_n(x) \propto e^{-nf(x)}, \quad x \in \mathbb{R}^d,$$

where sample size n and dimension d are both large, with $d = o(n)$. Standard Gaussian Laplace approximations are rigorously justified only in the regime $d = o(\sqrt{n})$, a condition that is too restrictive for many high-dimensional Bayesian problems. I will present a higher-order Laplace theory that remains valid arbitrarily close to the concentration threshold $d = o(n)$.

Under local smoothness and mild global growth assumptions, we derive explicit asymptotic expansions for normalizing constants and posterior expectations, with error of order d^{L+1}/n^L at expansion order L . These results provide a rigorous justification for higher-order corrections beyond the classical Gaussian approximation and substantially enlarge the range of dimensions for which Laplace-type approximations remain accurate.

I will also discuss sampling from concentrated posteriors π_n . We construct explicit polynomial transport maps that push forward a Gaussian reference measure to approximations of the posterior, with total variation error again of order d^{L+1}/n^L . Thus, by increasing the expansion order, both approximation and sampling remain accurate in regimes arbitrarily close to $d = o(n)$.

Overall, this work gives a rigorous and complete framework for the approximation and sampling of concentrated posterior distributions in growing dimension to arbitrary accuracy.

Wednesday June 10th – 1, 11:30 – 12:00, JCMB Lecture Theatre C

On the Algorithmic and Theoretical Path Towards Optimal Personalised Treatment

Session: Gradient Flows and Continuous-time Markov Processes in Data Science and Beyond p. 48

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Tailoring medical treatment strategies to the covariates of specific patient subgroups or even to individuals through simultaneous state and parameter estimation combined with Monte Carlo tree search strategies has shown highly promising results in improving therapeutic outcomes. An essential mathematical building block of these techniques is

access to a dynamic model that describes disease progression and the influence of control variables. If such a model is not available, it becomes necessary to identify or learn the causal relationships between medical interventions, patient covariates, and disease progression or improvement, and to construct a model from scratch—for example, using nonlinear mixed-effects compartment models such as PK/PD models. Once these relationships have been established and a patient-specific model is available, sequential filtering or smoothing approaches can be employed to assimilate incoming patient data and integrate it with model predictions. This creates a foundation for adaptive treatment policies, accounting for high individuality. Framing the dosing strategy as a sequential decision-making system induces a state to action mapping. With use of deep reinforcement learning methods in a Model-Informed Precision Dosing scenario we can propose therapeutic guidelines.

Our algorithmic pipeline showcases promising potential on recovering expert knowledge with inverse reinforcement learning.

Wednesday June 10th – 1, 11:30 – 12:00, JCMB 5326

Stochastic Optimal Control for a System of Delay Equations arising from Heat and Humidity Control

Session: Recent advances in hierarchical methods for uncertainty quantification, Part 1 p. 49

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The design of air conditioning systems in large buildings, including airports, or sensitive pharmaceutical laboratories requires high precision in both the calculation and evaluation of environmental conditions. Having in mind that probes in these laboratories need to undergo processes with strict temperature and humidity conditions requires accurate control of at least the air-conditioning (AC) systems responsible to make sure that the last two factors are in the acceptable regime. The warm-up time of the device poses mathematical challenges. It is physical to assume that to bring the environmental parameters into the acceptable regime, the AC system needs to be switched on for a certain amount of time. This period introduces a non-Markovian effect into the overall dynamics, giving rise to a system of controlled delay equations. We approximate solutions to these systems, after appropriate state augmentation, with a regression-based algorithm, and provide the relevant convergence theory.

Wednesday June 10th – 1, 12:00 – 12:30, JCMB Lecture Theatre A

The Tamed Subgradient Unadjusted Langevin Algorithm beyond Convexity

Session: Stochastic computation and complexity, Part 4

p. 47

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We study the problem of sampling from target distributions whose potentials are simultaneously non-smooth, subject to superlinear gradient growth, and non-convex. We introduce the Subgradient Tamed Unadjusted Langevin Algorithm (SG-TULA), a discretisation of the Langevin diffusion that operates directly on subgradients, without relying on computationally demanding smoothing procedures. To handle the superlinear regime, taming techniques are employed to produce a stable, explicit scheme. We derive non-asymptotic convergence bounds in Wasserstein-2 distance, with all constants tracked explicitly in terms of dimension and inverse temperature, improving upon the currently known rates for subgradient-based Langevin algorithms. We further provide excess risk estimates for the associated optimisation problem. Numerical experiments validate the theoretical findings and demonstrate competitive empirical performance against widely used adaptive optimisation algorithms, which have not been shown to admit comparable non-asymptotic guarantees in this setting.

Wednesday June 10th – 1, 12:00 – 12:30, JCMB Lecture Theatre B

Wasserstein Stability of Bayesian Posteriors in the Concentrated Posterior Regime

Session: Approximation and sampling of concentrated posterior distributions p. 47

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Understanding the stability of Bayesian posterior distributions under perturbations of the data is a classical problem in inverse problems and uncertainty quantification. This talk develops a Wasserstein-based perspective in regimes where the posterior concentrates, such as the small noise or large data setting.

While established bounds ensure local stability of the posterior under variations of the likelihood, the associated constants deteriorate in the concentration regime. In contrast, we show that, under standard assumptions, the Wasserstein distance between posterior distributions associated with different datasets admits a decomposition into the Euclidean distance between the corresponding maximum a posteriori estimators and a remainder of the order of the posterior contraction rate.

The framework applies both to the small noise setting and to large data regimes in which the likelihood evolves with increasing observations, and allows for multimodal posterior distributions. These results offer a perspective on posterior stability in the concentration regime that is relevant across a wide range of inverse problems.

Wednesday June 10th – 1, 12:00 – 12:30, JCMB Lecture Theatre C

Piecewise Deterministic Sampling for Constrained Distributions

Session: Gradient Flows and Continuous-time Markov Processes in Data Science and Beyond p. 48

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Sampling under constraints remains a challenging problem in high-dimensional settings and is of particular interest in a number of applications such as statistical mechanics [1] and inverse problems [2]. In this talk, we will discuss a novel class of piecewise deterministic Markov processes (PDMPs) that are designed to sample from constrained probability distributions π supported on a convex set \mathcal{M} . Our approach adapts the concept of a mirror map from convex optimisation to address the constrained sampling problem. This construction enables the development of unbiased algorithms that respect the constraints and allows for exact subsampling making them suitable for large-scale problems where processing the full dataset at every iteration is prohibitive. We provide theoretical guarantees for our proposed method and discuss conditions under which our constructed process is ergodic. We demonstrate the advantages of the proposed method on a range of constrained sampling problems. Empirical results show that our method outperform state of the art stochastic differential equation-based approaches in terms of sampling efficiency and accuracy, particularly in high dimensional settings.

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Wednesday June 10th – 1, 12:00 – 12:30, JCMB 5326

Multilevel Markov chain Monte Carlo for a class of partially observed diffusions with noiseless observations

Session: Recent advances in hierarchical methods for uncertainty quantification, Part 1
p. 49

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We consider Bayesian estimation of partially observed diffusion processes and their associated parameters, focusing on scenarios where data is recorded at regular and low-frequency intervals as linear and noiseless functions of the state at specific time points. This problem is particularly challenging because it constrains the diffusion process at observation times to particular manifolds defined by the data. Additionally, in many applications, it is necessary to discretize the diffusion process over time, which adds another layer of complexity. Using the antithetic weak order 2 time discretization presented in [1], we develop new antithetic multilevel Markov chain Monte Carlo algorithms to estimate expectations of the posterior distribution. Our methodology is applicable to both elliptic and hypoelliptic diffusion processes and is optimal under certain assumptions. Specifically, we achieve a mean square error in estimation of $\mathcal{O}(\epsilon^2)$ for a given $\epsilon > 0$, while the computational effort required to attain this is $\mathcal{O}(\epsilon^{-2})$.

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Wednesday June 10th – 2, 10:30 – 11:00, JCMB 5327

Energies with Tensor Product Structure, Fibonacci Lattices, and One-Distance Sets on the Torus

Session: Sample Points: Quality Measures, Constructions, and Applications p. 49
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We study minimizers of interaction energies on the flat torus \mathbb{T}^d , where the underlying kernel has tensor product structure. For N points $X = \{\mathbf{x}^0, \mathbf{x}^1, \dots, \mathbf{x}^{N-1}\} \subset \mathbb{T}^d \simeq [0, 1]^d$ with components $\mathbf{x}^k = (x_1^k, \dots, x_d^k)$, we define the *tensor product energy* as

$$E_F(X) = \sum_{\substack{k, \ell=0 \\ k \neq \ell}}^{N-1} F(\mathbf{x}^k - \mathbf{x}^\ell) = \sum_{\substack{k, \ell=0 \\ k \neq \ell}}^{N-1} \prod_{i=1}^d f(x_i^k - x_i^\ell),$$

where $f : \mathbb{R} \rightarrow \mathbb{R}_+$ is an even 1-periodic function. Such energies arise naturally in discrepancy theory (Warnock-type formulas) and quasi-Monte Carlo integration. Permutation sets on \mathbb{T}^2 and Latin hypercube sets in higher dimensions (i.e. sets whose projections onto coordinate axes are equispaced points) are natural candidates to be energy minimizers. We show that point configurations that have only one distance vector minimize the energy for a wide range of potentials, in other words, such sets exhibit a tensor product version of universal optimality. This applies, in particular, to three- and five-point Fibonacci lattices. We also characterize all lattices with this property and produce some non-lattice sets of this type. In addition, we discuss several further structural results about global and local minimizers of tensor product energies, in particular, for low values of N , as well as the closely related one-dimensional question (when do N equispaced points on the circle minimize the energy?) which surprisingly is still not completely understood.

Wednesday June 10th – 2, 10:30 – 11:00, JCMB 5328

Hierarchal Methods for Semilinear Stochastic Partial Differential Equations

Session: MLMC for SPDEs p. 50

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Multilevel and multi-index Monte Carlo (MLMC and MIMC) methods are highly efficient tools for uncertainty quantification, but their rigorous analysis and application have largely been confined to finite-dimensional stochastic differential equations (SDEs). Extending these frameworks to infinite-dimensional stochastic partial differential equations

(SPDEs), with their notoriously low regularity, introduces new challenges in discretization, coupling, and complexity analysis.

This talk first presents a multilevel Monte Carlo method based on a truncated Milstein-type scheme with antithetic coupling, extending the antithetic Milstein approach from SDEs to Hilbert space-valued SPDEs with non-commutative noise. The method retains the advantages of Milstein discretizations without requiring Lévy area terms, achieves enhanced variance decay, and maintains unbiasedness, resulting in reduced computational complexity.

The second part introduces a multi-index Monte Carlo method for semilinear parabolic SPDEs, built upon an exponential integrator and a multiplicative convergence property for coupled solutions. This construction leads to optimal asymptotic complexity and shows clear computational advantages over standard MLMC, especially in low-regularity settings.

Together, these results extend multilevel and multi-index methodologies beyond the finite-dimensional setting, offering efficient and analytically grounded approaches for high-dimensional stochastic systems.

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<https://doi.org/10.48550/arxiv.2502.00393>

[2] Haji-Ali, A.-L., & Stein, A. (2025). An Antithetic Multilevel Monte Carlo-Milstein Scheme for Stochastic Partial Differential Equations with non-commutative noise. *ESAIM: Mathematical Modelling and Numerical Analysis*, 59(3), 1437–1470.

<https://doi.org/10.1051/m2an/2025031>

Wednesday June 10th – 2, 10:30 – 11:00, JCMB 6206

Decision-making on a critical system using a rare event splitting technique

Session: Rare Events

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The reliability assessment of a critical industrial system (such as a power plant) can be performed based on an analysis of uncertainties and, ultimately, on the estimation of a *risk measure* characterizing the risk of the system failure. This estimate can be obtained using a numerical simulator $X \mapsto Y := g(X)$ that models the behavior of the system in its environment. The risk measures generally used correspond to an exceedance (or failure) probability $p_s := \mathbb{P}(Y > s)$ or a high-order quantile $q_{1-\alpha} := \inf \{y \in \mathbb{R} \mid \mathbb{P}(Y \leq y) \geq 1 - \alpha\}$, where $s \in \mathbb{R}$ is a safety threshold and $0 < \alpha < 1$ is an acceptable risk, both chosen in advance. The two following issues may then arise. (i) Because the system under study is critical, meaning the consequences of a failure would be dramatic, the sought failure probability is very small (respectively the quantile very high). As a consequence, the estimation of these quantities meets difficulties because of this *rare event* framework, especially when the numerical simulator g is costly to evaluate. (ii) Besides, in addition to estimation, another key task is to certify that these quantities are small enough [2, 4].

In this work, a statistical hypothesis test is proposed to guarantee the reliability of the system. Since we aim at proving the safety, the null hypothesis corresponds to the case where the system is unsafe. More precisely, this corresponds to situations where the failure probability is above some acceptable risk α , or equivalently, where the quantile is above the safety threshold s : $H_0 := \{p_s > \alpha\} = \{q_{1-\alpha} > s\}$ [2, 4]. The rejection region W of this statistical test depends on the number of iterations performed in a splitting technique, known as the *moving particles* algorithm [1, 5]. In this algorithm, a group of k particles of the input distribution X is iteratively moving towards the higher realizations of the output $Y = g(X)$. It relies on the ability to sample conditionally on the output of the numerical simulator, i.e. according to $(X|g(X) > y)$. Then the probability $\mathbb{P}(W)$ of rejecting the null hypothesis H_0 can be explicitly computed in terms of the true failure probability p_s , as illustrated in Figure 2. Moreover, under the null hypothesis H_0 , this rejection probability $\mathbb{P}_{H_0}(W)$ is always bounded by some $0 < \beta < 1$ chosen in advance. In practice, a standard approach is to approximate such conditional sampling using a Markov chain Monte Carlo (MCMC) technique. This work also explores the impact of the numerical approximation of this sampling on the aforementioned theoretical guarantees.

The statistical test developed shows several advantages. First, in its idealized version, it provides non-asymptotical guarantees, meaning that the probability $\mathbb{P}_{H_0}(W)$ of wrongly rejecting the null hypothesis H_0 can be as small as desired, based on a trade-off with numerical cost. Moreover, by comparison with a more standard test using classical Monte Carlo failure probability estimator [4], the proposed approach requires far fewer simulation code calls. Last but not least, because the test does not require to estimate the failure probability, the order of magnitude of the maximum number of code calls performed to reject the null hypothesis can be known beforehand, while it is not the case when directly estimating the failure probability using the *moving particles* algorithm.

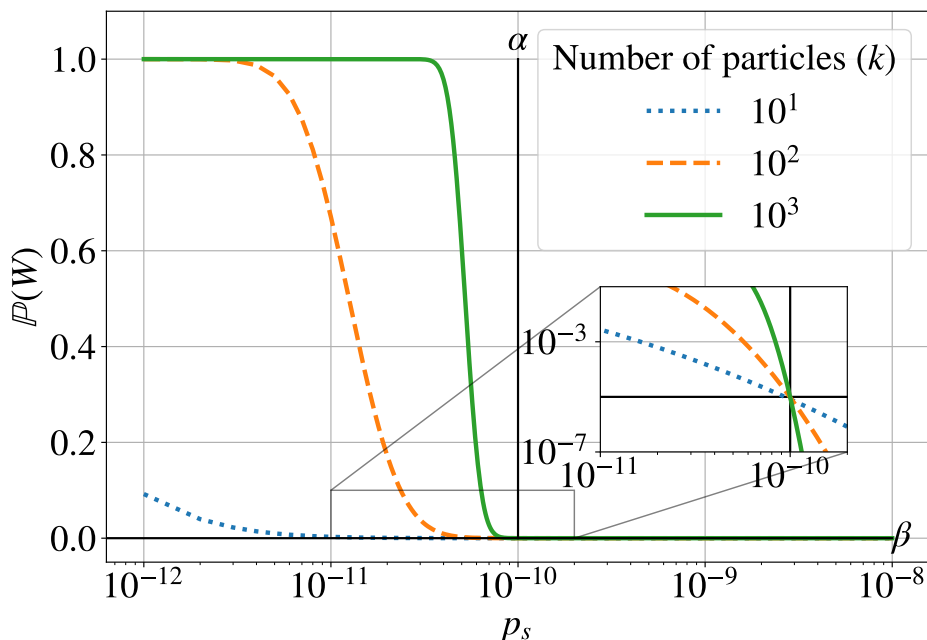


Figure 2: Probability of rejecting the null hypothesis $H_0 := \{p_s > \alpha\}$, with respect to the true (but unknown) failure probability p_s . When $p_s > \alpha$, then this rejection probability $\mathbb{P}(W)$ is always below β . When $p_s < \alpha$, this rejection probability is not necessarily close to 1, but it increases with the number of particles k .

As a perspective, some generalizations of this work could be of interest. The development of a similar decision-making framework based on importance sampling estimators instead of splitting techniques might be promising. Besides, in this work, the system is considered safe based on a failure probability (or equivalently a quantile) of the output. Yet, other risk measures could be used [4] such as the superquantile $\bar{q}_{1-\alpha} := \mathbb{E}(Y|Y > q_{1-\alpha})$, partly because of its relevant mathematical properties in the context of reliability assessment [3, 4].

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Wednesday June 10th – 2, 11:00 – 11:30, JCMB 5327

Optimality of quasi-Monte Carlo methods and suboptimality of the sparse-grid Gauss–Hermite rule

Session: Sample Points: Quality Measures, Constructions, and Applications p. 49
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Abstract: Computing integrals with respect to the Gaussian measure is a common task across many disciplines. In this talk, I will discuss optimal numerical integration rules for such a task. To formalise optimality, we fix a target function class and consider the L^2 -Sobolev space of dominating mixed smoothness.

In one dimension, the trapezoidal rule is asymptotically optimal in this space, up to a logarithmic factor. By contrast, Gauss–Hermite quadrature converges at only half this rate. A similar pattern holds for analytic functions.

We show that these results extend to higher dimensions: several quasi-Monte Carlo methods achieve the optimal rate, whereas the sparse-grid Gauss–Hermite rule based on attains only half the optimal rate.

Wednesday June 10th – 2, 11:00 – 11:30, JCMB 5328

Sampling the “same” coloured noise on different grid levels*Session: MLMC for SPDEs*

p. 50

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When simulating random fields or solutions to stochastic partial differential equations, an essential ingredient is the generation of the coloured spatial noise on a finite element space based on a grid. While this can already be a challenge, an additional interesting question comes up, when you want to computationally show strong convergence rates or apply a multilevel Monte Carlo scheme. These simulations require to generate the “same” noise sample on different spatial grid resolutions. In this talk, I will discuss what we mean by the “same” noise and introduce sampling methods.

Wednesday June 10th – 2, 11:00 – 11:30, JCMB 6206

Sequentially Adaptive Emulators for Rare Event Estimation*Session: Rare Events*

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The estimation of rare-event probabilities is a challenging problem in uncertainty quantification. Subset simulation is a powerful tool for this task; however, it requires repeated evaluations of the performance function and becomes computationally prohibitive when each evaluation is expensive. Surrogate modelling can reduce this computational cost by approximating the original performance function, but it may still require a large number of updates to ensure accuracy in rare-event regions. An active learning approach is proposed, combining a sequential Monte Carlo (SMC) sampler with Gaussian process (GP) emulators to provide a less expensive surrogate with uncertainty quantification. An SMC sampler with tempering proposals is used to select multiple new training samples per iteration, enabling efficient exploration of potentially disconnected rare-event regions. Iterative updates of the emulator and intermediate thresholds progressively refine the rare-event domain and ensure an accurate probability estimate at a reasonable computational cost. The method is demonstrated on numerical models and a cardio-respiratory model for intensive care unit patients.

Wednesday June 10th – 2, 11:30 – 12:00, JCMB 5327

Multi-fidelity quasi-Monte Carlo*Session: Sample Points: Quality Measures, Constructions, and Applications*

p. 49

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Multi-fidelity Monte Carlo (MFMC) has been successfully applied in many settings where a collection of models with varying cost and accuracy are combined to reduce variance at fixed computational budget. Building on this idea, we introduce a multi-fidelity variant of randomized quasi-Monte Carlo (MFQMC) that couples surrogate models with embedded lattice rules while preserving the unbiasedness and proven convergence properties of QMC.

Wednesday June 10th – 2, 11:30 – 12:00, JCMB 5328

Different MLMC treatments of the stochastic heat equation

Session: MLMC for SPDEs

p. 50

Mike Giles

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In this talk we consider three different treatments (spectral, finite element and finite volume) of the noise term in the stochastic heat equation, and use Fourier analysis to determine the MLMC correction variance for three different outputs, the squared amplitude of a single Fourier mode, the energy and the variance of a linear functional.

Key observations are that 1) the finite volume treatment has poorer variance, 2) Richardson extrapolation is needed to benefit fully from the improved spectral and finite element variance, 3) in all cases, the order of MLMC variance is much better than suggested by analysis based on the strong order of convergence.

Wednesday June 10th – 2, 11:30 – 12:00, JCMB 6206

Wasserstein Distributionally Robust Rare-Event Simulation

Session: Rare Events

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Standard rare-event simulation techniques require exact distributional specifications, which limits their effectiveness in the presence of distributional uncertainty. To address this, we develop a novel framework for estimating rare-event probabilities subject to such distributional model risk. Specifically, we focus on computing worst-case rare-event probabilities, defined as a distributionally robust bound against a Wasserstein ambiguity set centered at a specific nominal distribution. By exploiting a dual characterization of this bound, we propose Distributionally Robust Importance Sampling (DRIS), a computationally tractable methodology designed to substantially reduce the variance associated with estimating the dual components. The proposed method is simple to implement and requires low sampling costs. Most importantly, it achieves *vanishing relative error*—the strongest efficiency guarantee that is notoriously difficult to establish in rare-event simulation. Our numerical studies confirm the superior performance of DRIS against existing benchmarks.

Wednesday June 10th – 2, 12:00 – 12:30, JCMB 5327

Doubling the convergence rate with kernel approximation

Session: Sample Points: Quality Measures, Constructions, and Applications p. 49

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This talk describes an approximation result, obtained in joint work with Vesa Kaarnioja (BIT Numerical Mathematics 2025), in which the proven L_2 convergence rate of kernel interpolation of a smooth function f (where the kernel K is the reproducing kernel of a Hilbert space H), is twice as fast as expected from the smoothness of H . An application is to the approximation of the dependence with respect to parameters in a parametric partial differential equation.

Wednesday June 10th – 2, 12:00 – 12:30, JCMB 6206

Rare-Event Simulation of Top- k Exclusion in Mean-Field Elo Rating Models

Session: Rare Events

Koen De Turck

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We study rare collective misranking events in large-scale Elo-type rating systems. Consider an N -player model with fixed latent skills, random pairwise matching, and logistic win probabilities. Ratings evolve via standard Elo updates, yielding an interacting stochastic particle system in \mathbb{R}^N . In a large-population, small-step regime, the empirical rating distribution converges to a deterministic McKean–Vlasov transport equation.

Our focus is the top- k exclusion event: at a fixed time horizon, none of the true top- k players appear among the rated top- k . This event represents a collective leaderboard failure and cannot be attributed to isolated atypical outcomes. Heuristically, its probability is expected to decay exponentially in N , suggesting an underlying path-space large deviation principle for the empirical measure.

We analyze structural features of fluctuation paths leading to top- k exclusion and identify reaction coordinates based on order-statistic gaps that capture progress toward the rare event. These coordinates motivate rare-event Monte Carlo estimators using adaptive multilevel splitting and genealogical particle (cloning) algorithms. Numerical experiments indicate substantial variance reduction compared to naive simulation and provide empirical evidence for exponential scaling in the population size.

This work illustrates how modern rare-event Monte Carlo techniques can be applied to quantify robustness properties of rating systems and to explore structured deviations in mean-field interacting dynamics.

Thursday June 11th – Morning/1, 10:30 – 11:00, JCMB Lecture Theatre A

Numerical Integration and its Complexity for Functions with Uniformly Bounded Derivatives

Session: Complexity of high-dimensional approximation

p. 51

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We present results, proof techniques and open problems concerning the complexity of computing the integral of a function f defined on $[0, 1]^d$ and assume that f and some derivatives of f are bounded in the L_∞ norm. The stress is on lower bounds and the construction of fooling functions. We prove that the complexity of integration increases at least linearly in the dimension for some small classes of analytic functions. We also discuss fooling functions and lower bounds for the case when only positive quadrature formulas are used and discuss techniques that work for L_q norms with $q < \infty$, but not for $q = \infty$.

Thursday June 11th – Morning/1, 10:30 – 11:00, JCMB Lecture Theatre B

The star discrepancy of a union of randomly digitally shifted Korobov (polynomial) lattice point sets depends polynomially on the dimension

Session: New developments in quasi-Monte Carlo methods, Part 1

p. 51

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The inverse of the star discrepancy, $N(\varepsilon, s)$, defined as the minimum number of points required to achieve a star discrepancy of at most ε in dimension s , is known to depend linearly on s . However, explicit constructions achieving this optimal linear dependence remain elusive.

In this talk we discuss point sets constructed as multiset unions of Korobov rank-1 lattice point sets modulo a prime N . We cover four distinct construction scenarios, combining either random or fixed integer generators with either continuous torus shifts or discrete grid shifts. We show that in all four cases, the star discrepancy is bounded by a term of order $\mathcal{O}(s \log(N)/\sqrt{N})$ with high probability, where N is the total number of points, and the implied constant in the big-O notation is independent of N and s . This implies that the inverse of the star discrepancy for these structured sets depends quadratically on the dimension s . While the proofs are probabilistic, our results significantly reduce the search space for optimal point sets from a continuum to a finite set of candidates parameterized by integer generators and random shifts. Similar results also holds for randomly digitally shifted Korobov polynomial lattice point sets.

Thursday June 11th – Morning/1, 10:30 – 11:00, JCMB Lecture Theatre C

Computing importance weights for Markov chain Monte Carlo via couplings: an application to f-divergence diagnostics

Session: Probabilistic couplings for the design and analysis of Monte Carlo methods p. 52

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A long-standing gap exists between the theoretical analysis of Markov chain Monte Carlo convergence, which is often based on statistical divergences, and the diagnostics used in practice. We introduce the first general convergence diagnostics for Markov chain Monte Carlo based on any f -divergence, allowing users to directly monitor, among others, the Kullback-Leibler and the χ^2 -squared divergences as well as the Hellinger and the total variation distances. Our first key contribution is a coupling-based "weight harmonization" scheme that produces a direct, computable, and consistent weighting of interacting Markov chains with respect to their target distribution. The second key contribution is to show how such consistent weightings of empirical measures can be used to provide upper bounds to f -divergences in general. We prove that these bounds are guaranteed to tighten over time and converge to zero as the chains approach stationarity, providing a concrete diagnostic.

[1] A. Corenflos and H.-D. Dau. A coupling-based approach to f -divergences diagnostics for Markov chain Monte Carlo. *Preprint*, arXiv:2510.07559.

Thursday June 11th – Morning/1, 10:30 – 11:00, JCMB 5326

Rendering volumes with bitmasks

Session: Practical aspects of Monte Carlo simulation in applications

p. 53

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In Monte Carlo path tracing, one encounters particles that alternate between free flight and instantaneous direction changes. An example is the photorealistic rendering of scattering media in computer graphics. To estimate the incident light at a point in space, many particle paths need to be traced. Constructing such random walks requires repeatedly sampling distances to the next interaction event according to the free-path distribution.

However, this process becomes computationally expensive in heterogeneous volumes, mainly due to latency caused by many random memory accesses.

To reduce this cost, we introduce a novel way of encoding collision probabilities that enables efficient sampling of distances from an approximate free-path distribution on the GPU. At its core, the method performs distance sampling through a combination of bitmask selection and bitwise operations. In particular, only a single contiguous memory region is accessed per distance sample. Replacing more accurate ray marching with our method for higher-order scattering often yields a favorable trade-off between accuracy

and performance, although the benefits depend on the characteristics of the volume. The best results are observed for highly scattering media without sharp boundaries, such as clouds, whereas visible errors occur when rendering dense media with sharp boundaries.

We believe that this method is of interest to the broader Monte Carlo community, particularly in the context of hardware-oriented approaches to generating particle random walks.

Thursday June 11th – Morning/1, 11:00 – 11:30, JCMB Lecture Theatre A

Approximation of differential entropy in Bayesian optimal experimental design

Session: Complexity of high-dimensional approximation

p. 51

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We present a method to approximate differential entropy, which is then used to maximize the expected information gain, commonly used in Bayesian Optimal Experimental Design (BOED). We consider the standard additive noise model

$$y = \mathcal{G}(x; \xi) + \varepsilon,$$

where $y \in \mathbb{R}^d$ is the observed data, \mathcal{G} denotes the forward map, $x \in \mathcal{X}$ is the quantity of interest, ξ is the design variable, and ε is the additive noise. We assume that ε is Gaussian and does not depend on the design ξ . We want to maximize expected information gain,

$$\begin{aligned} U(\xi) &:= \iint_{\mathbb{R}^d \times \mathcal{X}} \left[\log \frac{\pi(y|x; \xi)}{\pi(y; \xi)} \right] \pi(x, y; \xi) dx dy \\ &= - \int_{\mathbb{R}^d} \log(\pi(y; \xi)) \pi(y; \xi) dy + \iint_{\mathbb{R}^d \times \mathcal{X}} \log(\pi(y|x; \xi)) \pi(y|x; \xi) dy \mu(x) dx \end{aligned}$$

where $\pi(x, y; \xi)$ stands for the joint distribution, $\pi(y|x; \xi)$ is the likelihood, $\pi(y; \xi)$ is the evidence, and $\mu(x)$ is the prior. In this setting, the second term above is independent of ξ . Thus we only need to maximize the first term, the differential entropy of the evidence.

We assume that evaluation of the forward map \mathcal{G} is the dominant cost of the problem, and we want to reduce the number of forward map evaluations, say M , as much as possible. To this end, we construct a surrogate model of the evidence $\pi(y; \xi)$. We show that our proposed method can attain the convergence rate $\mathcal{O}(M^{-1/2})$, and this can be accelerated by quasi-Monte Carlo methods. We also numerically demonstrate our method for a PDE problem where the dimensionality of \mathcal{X} is high.

Thursday June 11th – Morning/1, 11:00 – 11:30, JCMB Lecture Theatre B

Space-filling lattice designs for computer experiments

Session: New developments in quasi-Monte Carlo methods, Part 1

p. 51

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Based on a recent preprint [1], this talk investigates the geometric properties of quasi-Monte Carlo (QMC) lattice point sets, integrating their covering and separation radii through the unified criterion of quasi-uniformity. While quasi-uniform point sets are highly desirable as space-filling designs for computer experiments, their explicit construction remains challenging. We propose two novel construction algorithms for rank-1 lattices. The first generates lattice point sets as an explicit approximation of quasi-uniform Kronecker sequences. As a key theoretical contribution, we prove that this explicit construction achieves an isotropic discrepancy of $O(N^{-1/d})$, matching the optimal asymptotic rate previously known only via non-constructive existence proofs. The second algorithm employs the Lenstra–Lenstra–Lovász (LLL) basis reduction algorithm on Korobov lattices to identify generating vectors that ensure quasi-uniformity. Finally, we demonstrate the practical efficacy of these new space-filling QMC designs through numerical experiments, including empirical comparisons in the context of Gaussian process regression for computer experiments.

[1] N. Sakai and T. Goda, Space-filling lattice designs for computer experiments, arXiv:2602.15390 (2026).

Thursday June 11th – Morning/1, 11:00 – 11:30, JCMB Lecture Theatre C

Scalable Langevin Monte Carlo Methods for Bayesian Inference

Session: Probabilistic couplings for the design and analysis of Monte Carlo methods p. 52

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We introduce Langevin Monte Carlo methods for estimating expectations of observables under high-dimensional probability measures. We discuss discretization strategies and Metropolization methods for removing bias due to discretization error. We then present a new unbiased method for Bayesian posterior means based on kinetic Langevin dynamics that combines advanced splitting methods with enhanced gradient approximations. Our approach avoids Metropolis correction by coupling Markov chains at different discretization levels in a multilevel Monte Carlo approach. Theoretical analysis demonstrates that our proposed estimator is unbiased, attains finite variance, and satisfies a central limit theorem. We prove similar results using both approximate and stochastic gradients and show that our method’s computational cost scales independently of the size of the dataset. Our numerical experiments demonstrate that our unbiased algorithm outperforms the “gold-standard” randomized Hamiltonian Monte Carlo.

[1] N. K. Chada, B. Leimkuhler, D. Paulin, P. A. Whalley. Unbiased kinetic Langevin Monte Carlo with inexact gradients. *Annals of Statistics*, 2026+.

Thursday June 11th – Morning/1, 11:00 – 11:30, JCMB 5326

Artificially reduced collisionality Monte Carlo, an approximation method for neutral particles in the plasma edge of a fusion reactor

Session: Practical aspects of Monte Carlo simulation in applications p. 53

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In this talk, we introduce a new asymptotic-preserving Monte Carlo (APMC) method that can efficiently simulate neutral particles in the plasma edge of a fusion reactor: Artificially Reduced Collisionality Monte Carlo (ARC-MC). Simulating such particles is computationally expensive in regions with high collision rates, as Monte Carlo methods need to resolve each collision. For our new scheme, we modify the particles so that they have reduced collisionality. Simply reducing the collisionality introduces a significant bias, so we also modify the velocity distribution to offset this bias. We will show in numerical experiments that ARC-MC is significantly more accurate than KDMC, another APMC method. We also incorporate ARC-MC into a multilevel Monte Carlo scheme and show that this is not only highly effective, but also easier to implement than multilevel KDMC.

Acknowledgements. This work has been carried out within the framework of the EUROfusion Consortium, funded by the European Union via the Euratom Research and Training Programme (Grant Agreement No 101052200 — EUROfusion). Views and opinions expressed are however those of the author(s) only and do not necessarily reflect those of the European Union or the European Commission. Neither the European Union nor the European Commission can be held responsible for them.

Thursday June 11th – Morning/1, 11:30 – 12:00, JCMB Lecture Theatre A

Instance optimal sampling recovery and minimal number of samples

Session: Complexity of high-dimensional approximation p. 51

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This talk concerns the reconstruction of multivariate functions from samples using sparse recovery techniques. We build upon the results from [1] and show that the main results there, bounding sampling numbers in L_2 from above by the best m -term approximation in L_∞ can be refined in two directions. First we observe that Square Root Lasso and Orthogonal Matching Pursuit instead of Basis Pursuit Denoising allows us to give instance optimal bounds. The deployed decoders require only a search space V_J spanned by dictionary elements indexed by J , and a sparsity parameter n instead of information on the function class, to guarantee an L_2 -approximation error decaying no worse than a best n -term approximation error as well as the truncation error with respect to the

search space V_J and the uniform norm. This happens simultaneously for all admissible functions if the number of samples scales as $n \log^2 n \log |J|$, based on known bounds for the RIP of matrices constructed from bounded orthonormal systems. In addition we can generalize these results to sampling numbers measured in L_q . We present applications of these general bounds and show results for sampling widths in certain function classes. Finally, we establish lower bounds on the required sample complexity, which show that the log-factor in $|J|$ is indeed necessary to obtain such *instance-optimal* error guarantees.

[1] T. Jahn, T. Ullrich, and F. Voigtlaender. Sampling numbers of smoothness classes via ℓ^1 -minimization. *Journal of Complexity*, 79:Paper No. 101786, 35, 2023.

Thursday June 11th – Morning/1, 11:30 – 12:00, JCMB Lecture Theatre B

Quasi-Monte Carlo for SDE Simulation: Error Analysis and Dimensionality Reduction

Session: New developments in quasi-Monte Carlo methods, Part 1

p. 51

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We investigate the numerical simulation of general stochastic differential equations (SDEs) using Quasi-Monte Carlo (QMC) methods. First, we provide a rigorous theoretical analysis of the QMC method applied to the Euler-Maruyama (EM) scheme, establishing that it significantly accelerates the decay of the sampling error and achieves an asymptotically superior convergence rate over the classical Monte Carlo method. Second, the traditional EM scheme exhibits a slow polynomial decay of the discretization error, which necessitates a large number of time steps and leads to a significantly high integration dimension. To address this issue, we propose a Multilevel Stochastic Time Grid (MSTG) method based on Exact Simulation techniques, and we rigorously establish its convergence rate under Randomized QMC sampling, proving that it preserves the high-order convergence of the sampling error. In terms of the overall error, the truncation error of the proposed MSTG method exhibits a remarkably fast super-exponential decay. Consequently, to achieve a given accuracy level, our approach requires significantly fewer discretization steps than the EM scheme, thereby drastically reducing the actual integration dimension of the QMC method. This substantial dimensionality reduction strategy enhances the practical efficiency of the QMC algorithm. Numerical experiments corroborate the superiority of the proposed approach.

Thursday June 11th – Morning/1, 11:30 – 12:00, JCMB Lecture Theatre C

Scaling couplings of Markov chain Monte Carlo algorithms to high dimensions

Session: Probabilistic couplings for the design and analysis of Monte Carlo methods p. 52

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Coupling methods have become an increasingly attractive tool for users of Markov chain Monte Carlo (MCMC): they offer principled efficiency diagnostics, unbiased estimation, and natural parallelism. Yet two fundamental questions remain underexplored — how well can these methods actually perform as the dimension of the target distribution grows, and how should one design couplings that recover near-optimal behaviour?

This talk addresses these questions for the random walk Metropolis (RWM) algorithm, one of the most popular and robust MCMC algorithms. Paradoxically, the simplicity of the RWM algorithm actively impedes the design of effective couplings — the symmetric proposal distribution lacks a clear mechanism to drift two coupled chains towards each other. We [1] reveal that coupled RWM chains can nevertheless contract by deriving appropriate high-dimensional limits, extending established results in the marginal case [2,3]. This insight allows us to devise practical couplings that recover the provably-optimal $\mathcal{O}(d)$ scaling of the RWM with the dimension d .

- [1] T. P. Papp and C. Sherlock. Scalable couplings for the random walk Metropolis algorithm. *Journal of the Royal Statistical Society: Series B*, 2025.
- [2] G. O. Roberts, A. Gelman, and W. R. Gilks. Weak convergence and optimal scaling of random walk Metropolis algorithms. *The Annals of Applied Probability*, 1997.
- [3] O. F. Christensen, G. O. Roberts, and J. S. Rosenthal. Scaling limits for the transient phase of local Metropolis–Hastings algorithms. *Journal of the Royal Statistical Society: Series B*, 2005.

Thursday June 11th – Morning/1, 11:30 – 12:00, JCMB 5326

Multifidelity Uncertainty Quantification for Photon Radiotherapy

Session: Practical aspects of Monte Carlo simulation in applications

p. 53

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During a radiotherapy treatment, large amounts of ionising radiation are delivered to a patient using machinery with finite precision. A key question is how sensitive the whole treatment process is to this machine uncertainty. Although the answer is case specific and computationally burdensome, parts of it have been incorporated into the clinical workflow. To speed up these calculations, this talk introduces the multifidelity framework by Peherstorfer and colleagues into the radiotherapy context. The multifidelity algorithm uses models of different accuracy and computational cost to calculate the expected value of quantities more efficiently.

Thursday June 11th – Morning/1, 12:00 – 12:30, JCMB Lecture Theatre A

L_2 -approximation using median lattice algorithms

Session: Complexity of high-dimensional approximation p. 51

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We study the problem of multivariate L_2 -approximation of functions in a weighted Korobov space. We propose a median lattice-based algorithm, inspired by median integration rules, which have attracted significant attention in the theory of quasi-Monte Carlo methods. Our algorithm approximates the Fourier coefficients associated with a suitably chosen frequency index set, where each coefficient is estimated by taking the median over approximations from randomly shifted rank-1 lattice rules with independently chosen generating vectors. We prove that the algorithm achieves, with high probability, a convergence rate of the L_2 -approximation error that is arbitrarily close to optimal with respect to the number of function evaluations. Furthermore, we show that the error bound depends only polynomially on the dimension, or is even independent of the dimension, under certain summability conditions on the weights. We also include the discussion of a “universal” variant of the algorithm, where we do not need prior information on smoothness and weights.

Thursday June 11th – Morning/1, 12:00 – 12:30, JCMB Lecture Theatre B

Convergence Analysis for Generative Models with Quasi-Monte Carlo Importance Sampling

Session: New developments in quasi-Monte Carlo methods, Part 1 p. 51

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High-dimensional numerical integration with respect to complex target measures remains a fundamental challenge in computational science. While deep generative models such as Flow Matching, Diffusion, and Normalizing Flows offer a powerful paradigm for constructing continuous-time transport maps, their deployment in high-precision numerical integration is often limited by discretization bias and the lack of rigorous convergence guarantees.

To address these critical gaps, we propose a unified theoretical framework that integrates these generative models with Quasi-Monte Carlo (QMC) methods and Importance Sampling (IS). Methodologically, we construct transport maps by composing a base transformation with flow mappings (e.g., Euler-discretized neural ODEs or autoregressive layers), and leverage importance sampling to correct the approximation bias of the learned maps, thereby ensuring an unbiased estimation framework.

Our central contribution is twofold. First, we establish a general convergence analysis for the randomized QMC (RQMC) Importance Sampling using transport maps, identifying sufficient boundary growth conditions that ensure high-order convergence. Second,

we rigorously prove that under certain assumptions on the neural network architectures, the specific transport architectures of Flow Matching, Diffusion, and Normalizing Flows inherently satisfy these conditions. Consequently, we establish that the resulting unbiased estimators achieve a root-mean-square error of order $\mathcal{O}(N^{-1+\epsilon})$, effectively extending classical QMC theory to the realm of deep generative modeling.

Thursday June 11th – Morning/1, 12:00 – 12:30, JCMB Lecture Theatre C

Mixing time of the conditional backward sampling particle filter

Session: Probabilistic couplings for the design and analysis of Monte Carlo methods p. 52

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The conditional backward sampling particle filter (CBPF) is a powerful Markov chain Monte Carlo sampler for general state space hidden Markov model (HMM) smoothing. We show that the CBPF has $O(T \log T)$ time complexity under strong mixing: its mixing time is upper bounded by $O(\log T)$, for any sufficiently large number of particles N independent of T . This $O(\log T)$ mixing time is optimal. To prove our main result, we introduce a novel coupling of two CBPFs, which employs a maximal coupling of two particle systems at each time instant. The coupling is implementable and we use it to construct unbiased, finite variance, estimates of functionals which have arbitrary dependence on the latent state's path, with a total expected cost of $O(T \log T)$. We use this to construct unbiased estimates of the HMM's score function, and also investigate other couplings which can exhibit improved behaviour.

[1] J. Karjalainen, A. Lee, S. S. Singh, M. Vihola. Mixing time of the conditional backward sampling particle filter. *Journal of the Royal Statistical Society: Series B*, 2025.

Thursday June 11th – Morning/1, 12:00 – 12:30, JCMB 5326

Reversing SPRNG: on Reversible Pseudorandom Number Generators

Session: Practical aspects of Monte Carlo simulation in applications

p. 53

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Pseudorandom number generators are normally initialized via some seeding procedure and then generate a stream of random numbers in a particular deterministic order. There are several applications where having the ability to take such a stream and generate it backwards is very useful. One such application is where a path-based estimator is generated and one seeks to replay the trajectory backwards from the original end point to the original starting point. In order to provide reversible random number generators, we have made several of The Scalable Parallel Random Number Generators (SPRNG) library [1] reversible. SPRNG is a popular tool that is used in Monte Carlo simulation that was developed in our group. This talk goes in the detail of how we made several of the SPRNG generators reversible and still maintain the reproducibility of SPRNG. Not all the generators in SPRNG are easily reversible and so we plan to release a reversible version of SPRNG in the near future that include only those generators that can practically be reversed.

[1] M. Mascagni and A. Srinivasan. “Algorithm 806: SPRNG”. In: ACM Transactions on Mathematical Software 26.3 (2000), pp. 436–461. DOI: 10.1145/358407.

Thursday June 11th – Morning/2, 10:30 – 11:00, JCMB 5327

Weak Poincaré inequalities for Deterministic-scan Metropolis-within-Gibbs samplers

Session: Recent Advances in Gibbs Sampling

p. 54

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Using the framework of weak Poincaré inequalities, we analyze the convergence properties of two-component deterministic-scan Metropolis-within-Gibbs samplers, an important class of Markov chain Monte Carlo algorithms. Our analysis applies to nonreversible Markov chains and yields explicit (subgeometric) convergence bounds through novel comparison techniques based on Dirichlet forms. In addition, we show that the joint chain inherits the convergence behavior of the marginal chain and conversely. We apply our theoretical results through applications to algorithms for a diffusion model under discretely-observed data, with particular focus on the Ornstein-Uhlenbeck process to obtain the explicit convergence bound.

Thursday June 11th – Morning/2, 10:30 – 11:00, JCMB 5328

Wasserstein de-initialization for Markov chains

Session: Markov chains and Monte Carlo

Mareike Hasenpflug

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The de-initializing framework proposed in [1] is a way of obtaining bounds on the convergence of a Markov chain in total variation distance. The main idea is to exploit relationships to “simpler” chains. In this talk we generalize the de-initializing framework

to Wasserstein distances, such that bounds for the Wasserstein convergence of a Markov chain can be obtained. We apply our results to get upper and lower bounds for different Markov chain Monte Carlo methods.

- [1] G. O. Roberts and J. S. Rosenthal. Markov chains and de-initializing processes. *Scandinavian Journal of Statistics*, 28(3):489–504, 2001.

Thursday June 11th – Morning/2, 10:30 – 11:00, JCMB 6206

A filtered multilevel Monte Carlo method for the normalization of diffusion-based covariance operators

Session: Multilevel Methods and PDEs

Paul Mycek

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Error covariance operators play a crucial role in data assimilation methods for combining the heterogeneous and uncertain information provided by models and observations to estimate the state and/or some parameters of a system.

Modern methods for modelling covariance operators include diffusion-based approaches, in which stationary stochastic fields with a Matérn-like covariance structure are approximated by a diffusion operator. Such diffusion-based covariance operators have the desired (approximate) covariance structure, but not the desired variances. To impose the correct variances, the diffusion-based covariance operator first needs to be normalized into a correlation operator, then scaled back to match the desired variances. One way to perform the normalization step consists in estimating the variance of a discretized random field by a Monte Carlo (MC) method.

In this work, we propose to improve the estimation via a multilevel Monte Carlo (MLMC) approach, thereby leveraging a hierarchy of discretization grids for solving the diffusion problems. The approach involves inter-grid (prolongation and restriction, in multigrid jargon) operators to transfer the input and output discretized fields from one level of discretization to the previous/next one in the grid hierarchy. We demonstrate numerically that these operators introduce spurious high-frequency components in the transferred signals, which in turn deteriorate the normwise variance of the resulting MLMC estimator, thus inhibiting its full potential.

We propose to introduce an inter-grid pre-restriction and post-prolongation filtering mechanism that effectively damps the spurious high frequencies and mitigates the overall variance degradation. The resulting filtered MLMC (F-MLMC) method is tested numerically on a 2D normalization problem and compared to its unfiltered counterpart. We discuss the design of the inter-grid transfer and filtering operator, and draw parallels with the weighted MLMC method, or more generally the multilevel best linear unbiased estimator (MLBLUE) approach.

Thursday June 11th – Morning/2, 11:00 – 11:30, JCMB 5327

On spectral decomposition for Markov chains*Session: Recent Advances in Gibbs Sampling*

p. 54

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I will present a framework encompassing a range of decomposition results for convergence analysis of Markov chains. This type of result factors the spectral gap of a complicated Markov chain into simpler components, facilitating the analysis of important MCMC algorithms like hybrid Gibbs samplers and reversible jump algorithms. I will explain how multiple existing decomposition results can be unified under the same framework, and present some new decomposition results derived from the framework.

Thursday June 11th – Morning/2, 11:00 – 11:30, JCMB 5328

Solving Poisson's equation for Wasserstein contractive Markov chains*Session: Markov chains and Monte Carlo*

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We study Poisson's equation in the context of general state space Markov chains. For chains satisfying a contraction assumption w.r.t. a Wasserstein distance we show that a solution exists for forcing functions which are Lipschitz. If the solution of Poisson's equation is sufficiently regular, then a martingale decomposition technique can be employed to investigate the convergence of empirical averages corresponding to the Markov chain. Examples from the Markov chain Monte Carlo (MCMC) literature which satisfy the contraction assumption are provided. In particular, this allows to deduce statements about the convergence of the corresponding MCMC estimators for numerical integration.

Thursday June 11th – Morning/2, 11:00 – 11:30, JCMB 6206

Single-ensemble multilevel simulation of McKean-Vlasov equations*Session: Multilevel Methods and PDEs*

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McKean–Vlasov equations are stochastic differential equations whose coefficients depend on the law of the solution. They describe the evolution of large systems of interacting particles and are widely used in physics, finance, and biology. Their simulation can be computationally expensive, as accurate approximations require large ensembles and fine time discretizations. A multilevel Monte Carlo method based on simulating

multiple independent ensembles with small time steps and large ensembles on finer levels, was introduced in [1]. In this talk, we present an alternative multilevel approach using a *single, globally-coupled ensemble*, which allows to decrease the subensemble size on higher levels, at the cost of cross-level dependencies. We will make an analytical and numerical comparison of both algorithms.

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Thursday June 11th – Morning/2, 11:30 – 12:00, JCMB 5327

Spectral gap of Metropolis-within-Gibbs under log-concavity

Session: Recent Advances in Gibbs Sampling

p. 54

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The Metropolis-within-Gibbs (MwG) algorithm is a widely used Markov Chain Monte Carlo method for sampling from high-dimensional distributions when exact conditional sampling is intractable. We study MwG with Random Walk Metropolis (RWM) updates, using proposal variances tuned to match the target’s conditional variances. Assuming the target is a d -dimensional log-concave distribution with condition number κ , we establish a spectral gap lower bound of order $O(1/\kappa d)$ for the random-scan version of MwG. The result shows that MwG can mix substantially faster with variance-adaptive proposals and that its mixing performance is just a constant factor worse than that of the exact Gibbs sampler, thus providing theoretical support to previously observed empirical behavior.

Reference:

[1] C. Secchi and G. Zanella (2025+) Spectral gap of Metropolis-within-Gibbs under log-concavity. Preprint at [arxiv:2509.26175](https://arxiv.org/abs/2509.26175)

Thursday June 11th – Morning/2, 11:30 – 12:00, JCMB 5328

On Monte Carlo with Global Proposals

Session: Markov chains and Monte Carlo

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We call *Monte Carlo with global proposals* any method that operates in three steps: (i) draw samples x_1, \dots, x_N from a proposal distribution q defined over the full state space, (ii) evaluate the importance weights

$$\omega(x) = \frac{\pi(x)}{q(x)},$$

which are the Radon–Nikodym derivative of the target π with respect to q , and (iii) combine these samples and weights to produce estimators or approximate samples from π . The term *global* distinguishes these proposals from *local* ones, such as random walk Metropolis, where q depends on the current state of the chain. Different choices in step (iii) give rise to different algorithms: this framework encompasses importance sampling (IS) [4], the independent Metropolis–Hastings algorithm (IMH) [3], and sampling importance resampling (SIR) [5]. These methods also serve as core subroutines in more elaborate algorithms such as sequential Monte Carlo, annealed importance sampling, and pseudo-marginal Markov chain Monte Carlo [1]; we briefly survey this broader landscape during the talk.

Under the assumption that the weight function is unbounded, i.e. $\sup_x \omega(x) = \infty$, but has finite moments under q , we study the approximation error of importance sampling and of the particle independent Metropolis–Hastings algorithm (PIMH) [1, 6], which includes IMH as a special case. For the chains generated by such algorithms, we show that the common random numbers coupling is maximal. Using that coupling we derive explicit bounds on the total variation distance of a PIMH chain to its target distribution at finite time n :

$$\text{TV}(\mathcal{L}(X_n), \pi) \leq C(N, n),$$

where N is the number of particles and $C(N, n)$ is made explicit. Our results allow a formal comparison of the finite-time biases of importance sampling and IMH, and we find the latter to have a smaller bias. We further consider bias removal techniques using couplings [2], and provide conditions under which the resulting unbiased estimators have finite moments. These unbiased estimators provide an alternative to self-normalized importance sampling, applicable in the same settings. We compare their asymptotic efficiency as $N \rightarrow \infty$, and consider their use in robust mean estimation techniques.

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Thursday June 11th – Morning/2, 11:30 – 12:00, JCMB 6206

Coarse-to-Fine Coupling for Accelerated Probabilistic Shape Modelling

Session: Multilevel Methods and PDEs

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Probabilistic diffeomorphic shape models provide uncertainty-aware representations of geometric variation, but fitting them is a demanding high-dimensional Bayesian inference problem. We consider Gaussian-process-driven flow-based models in which shapes arise as diffeomorphic deformations of a template under time-dependent vector fields. Fitting is performed by variational inference (VI) and requires Monte Carlo (MC) gradient estimates of expectations under variational posteriors. In high dimensions, these estimators can be both computationally expensive and high-variance, and naive multiscale schemes may lose accuracy when coarse and fine dynamics are only weakly coupled.

We propose a coarse-to-fine multilevel framework that couples variational approximations and MC sampling across subspaces. The method constructs deformation-aware coarsening operators and a lifting procedure embedding the coarse model and variational GP components into a fine subspace, while enforcing shared randomness and coupled variational distributions across levels. As a result, paired coarse and fine samples are strongly correlated, producing tightly coupled vector fields and deformation trajectories. The lifted coarse model also provides a consistent fine-level initialisation, reducing expensive fine-resolution optimisation. We support the method with theoretical analysis and numerical examples, and observe at least a twofold reduction in wall-clock time compared with standard single-level variational fitting, without loss of deformation fidelity.

Thursday June 11th – Morning/2, 12:00 – 12:30, JCMB 5328

RQMC for Confidence Intervals using a Bounded Kurtosis Assumption

Session: Markov chains and Monte Carlo

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Hickernell et. al [1] derived a finite sample confidence interval for the mean of a random variable Y based on independent and identically distributed (IID) random samples of Y , which assumes a bound on the kurtosis of Y . To apply their finite sample CI to randomized quasi-Monte Carlo (RQMC), we take R independent replications of n RQMC points, averaging the n function evaluations within each replication. We have currently made use of Nested Uniform Scrambling with Faure sequence as the kurtosis (the fourth standardized moment) approaches 3 for large n , having nearly a Gaussian distribution. However, it's also interesting to explore other low-discrepancy sequences and randomizations.

Hickernell et. al [1] use two independent samples of Monte Carlo points. Here we use two independent sets of RQMC replicates. The first set, S_1 , contains $R_1 \geq 2$ independent draws from the integrand and the second set, S_2 , contains $R_2 \geq 1$ independent draws from the integrand. Both use the same n . All $R_1 + R_2$ RQMC estimates are independent.

S_1 is used to derive a bound on the variance σ_n^2 with a factor of safety $F > 1$ and requires a large R_1 . S_2 uses R_2 replications to deliver an estimate $\hat{\mu}$ with

$$\Pr(|\hat{\mu} - \mu| \leq \varepsilon) \geq 1 - \alpha$$

where μ is the integral expectation, $\varepsilon > 0$ is the uncertainty requirement and $\alpha \in (0, 1)$ is the error probability. For S_2 , various methods like Chebychev, Berry-Esseen, Catoni, median of means, etc. can be used to deliver the estimate $\hat{\mu}$ and we can pick the one giving the smallest R_2 .

It's crucial to ensure the kurtosis is bounded for finite n . We make use of extensive simulations for ridge functions with varying smoothness to ensure we get modest kurtoses for different dimensions, n , and smoothness. We are also interested in seeing whether these confidence intervals give us atleast the desire confidence level α , something requiring at least a 1000 trials of our experiments.

- [1] F. J. Hickernell, L. Jiang, Y. Liu, and A. B. Owen. Guaranteed conservative fixed width confidence intervals via Monte Carlo sampling. In J. Dick, F. Y. Kuo, G. W. Peters, and I. H. Sloan, editors, Monte Carlo and Quasi-Monte Carlo Methods 2012, volume 65 of Springer Proceedings in Mathematics and Statistics, pages 105–128. Springer-Verlag, Berlin, 2013.

Thursday June 11th – Morning/2, 12:00 – 12:30, JCMB 6206

Gevrey class and beyond in PDE uncertainty quantification

Session: Multilevel Methods and PDEs

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There has been a surge of interest in uncertainty quantification for parametric partial differential equations (PDEs) with Gevrey regular random field inputs. The Gevrey class consists of functions that are infinitely smooth with a growth condition placed on the higher-order partial derivatives, but which are nonetheless not analytic in general. In this talk, we explore a generalization of the Gevrey class for parametric inputs, obtained by composing a Gevrey regular parameterization of a random input with a nonlinear change of variables. We show that such a model admits dimension-independent quasi-Monte Carlo convergence rates within the context of PDE uncertainty quantification. Furthermore, we derive explicit rates for the dimension truncation error in this setting.

Thursday June 11th – Afternoon/1, 15:30 – 16:00, JCMB Lecture Theatre A

Good Lattice and Kronecker Sequences for Arbitrary Sample Size

Session: Stochastic computation and complexity, Part 6

p. 54

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Low discrepancy sequences used for quasi-Monte Carlo computations are often optimized for a sequence of sample sizes, such as powers of a prime base. This is particularly true for lattices and digital sequences. While the preferred sample sizes are best, the user might not be able to fully control the node set because of budget constraints or missing data. We explore how well one can do for arbitrary sample sizes, in particular for lattices and Kronecker sequences. We derive a weighted sum of squared expected discrepancies over all sample sizes as our figure of merit. We use component-by-component constructions to obtain new low discrepancy sequences.

Thursday June 11th – Afternoon/1, 15:30 – 16:00, JCMB Lecture Theatre B

Nested Multilevel Monte Carlo with Preintegration for Efficient Risk Estimation

Session: New developments in quasi-Monte Carlo methods, Part 2 p. 55

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Nested Monte Carlo is widely used for risk estimation, but its efficiency is limited by the discontinuity of the indicator function and high computational cost. This paper proposes a nested Multilevel Monte Carlo (MLMC) method combined with preintegration for efficient risk estimation. We first use preintegration to integrate out one outer random variable, which effectively handles the discontinuity of the indicator function, then we construct the MLMC estimator with preintegration to reduce the computational cost. Our theoretical analysis proves that the strong convergence rate of the MLMC combined with preintegration reaches -1 , compared with $-1/2$ for the standard MLMC. Consequently, we obtain a nearly optimal computational complexity. Besides, our method can also handle the high-kurtosis phenomenon caused by indicator functions. Numerical experiments verify that the smoothed MLMC with preintegration outperforms the standard MLMC and the optimal computational cost can be attained. Combining our method with quasi-Monte Carlo further improves its performance in high dimensions.

Thursday June 11th – Afternoon/1, 15:30 – 16:00, JCMB Lecture Theatre C

High-Dimensional Bayesian Level Set Inversion in Time-Domain Acoustic Waves

Session: Bayesian inference using Monte Carlo and quasi-Monte Carlo methods p. 55

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Reconstructing the velocity of seabed displacement from indirect measurements is a central task in early tsunami detection. Pressure measurements in the ocean provide a promising approach, due to the faster propagation of acoustic waves compared to tsunami water waves [1]. We formulate this problem as a high-dimensional Bayesian inverse problem.

We introduce a statistical and physical model in which the seabed velocity is represented through a level set prior [2], entering as a boundary condition in a time-domain acoustic wave equation. To mitigate spurious oscillations arising from the pressure time series data, we employ a Wasserstein log-likelihood [3].

We then address the well-posedness of the resulting Bayesian inverse problem, where the main challenge arises from the low spatial regularity induced by the level set prior.

Finally, we discuss sampling from the posterior and present numerical experiments demonstrating the feasibility of the approach, as well as the impact of wave propagation physics on the reconstruction.

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Thursday June 11th – Afternoon/1, 16:00 – 16:30, JCMB Lecture Theatre A

Gibbsian polar slice sampling

Session: Stochastic computation and complexity, Part 6

p. 54

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Gibbsian polar slice sampling, a Markov chain Monte Carlo method for approximate sampling of distributions only known up to normalizing constants, is able to perform well in high-dimensional settings and heavy-tailed scenarios. The aim of the presentation is to provide an introduction to the sampling scheme as well as to point to recent theoretical developments. Specifically, we show dimension-robust spectral gap estimates of the corresponding Markov operator which yield, under appropriate assumptions, dimension-independent convergence guarantees.

Thursday June 11th – Afternoon/1, 16:00 – 16:30, JCMB Lecture Theatre B

Quasi-Monte Carlo with a Hankel random digital net

Session: New developments in quasi-Monte Carlo methods, Part 2

p. 55

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This paper proposes a new randomized design of digital nets in which the generating matrices are chosen to be random Hankel matrices. Compared with previous randomized design of digital nets, this approach simplifies the construction process and reduces the number of random variables required, while still achieving desirable convergence rates when combined with appropriate estimators. We analyze the properties of the proposed design, derive bounds for Walsh coefficients, and provide error analysis for both the median-of-means estimator and a newly proposed greedy selection estimator, i.e. the selection of the best design from a batch in terms of a worst-case error bound. Numerical experiments validate our theoretical findings and demonstrate the practical performance of the proposed methods.

Thursday June 11th – Afternoon/1, 16:00 – 16:30, JCMB Lecture Theatre C

Fast Bayesian shape parameter estimation for parabolic PDEs in moving domains

Session: *Bayesian inference using Monte Carlo and quasi-Monte Carlo methods* p. 55

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We study the shape inversion problem for linear parabolic PDEs in random non-cylindrical domains under general parametrizations. This is framed as a Bayesian parameter estimation problem, where the parameters control the shape of the domain and/or the velocity field. We employ unfitted space-time finite elements to discretize the solutions to the PDEs and design quasi-Monte Carlo rank-1 lattice rules for the approximation of moments of the posterior. Combining these with a Laplace approximation of the resulting high-dimensional integrals, we give a full convergence analysis of the problem. Numerical experiments are included to verify the results.

Thursday June 11th – Afternoon/1, 16:30 – 17:00, JCMB Lecture Theatre A

Optimality of QMC Quadrature Rules on Multiple Scales of Function Spaces

Session: *Stochastic computation and complexity, Part 6* p. 54

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We study the integration problem over the d -dimensional unit cube on three scales of Banach spaces of integrands. We analyze quasi-Monte Carlo (QMC) quadrature rules based on arbitrary (t, m, d) -nets and on Halton sequences. We derive upper bounds and matching lower bounds for their worst-case errors over the norm unit balls of Haar wavelet

spaces, which consist of functions whose Haar wavelet coefficients exhibit a certain decay behavior.

We discuss several suitable function space embeddings that allow to transfer our upper error bounds from Haar wavelet spaces to Besov and to Sobolev spaces of dominating mixed smoothness less than one. Known lower bounds for arbitrary quadrature rules on those Besov and Sobolev spaces show that QMC quadratures based on (t, m, d) -nets and on Halton sequences yield optimal convergence rates also on these two scales of function spaces.

A major part of the talk is based on the following two references.

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Thursday June 11th – Afternoon/1, 16:30 – 17:00, JCMB Lecture Theatre B

Randomized Quasi-Monte Carlo for Walk on Spheres

Session: New developments in quasi-Monte Carlo methods, Part 2

p. 55

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Walk on Spheres (WOS) is a grid-free Monte Carlo method for estimating solutions to boundary value problems via probabilistic representations [1]. Rather than simulating full Brownian paths, WOS iteratively samples exit points from the largest sphere contained in the domain and centered at the current location. The walk stops when it enters a small boundary neighborhood, and the boundary data are evaluated at the projected terminal point. Averaging over many independent walks produces an estimator of the solution.

In this project, we replaced standard Monte Carlo sampling within WOS by randomized quasi-Monte Carlo (RQMC) point sets and study the resulting error and variance behavior. Across a range of test problems and geometries, including examples drawn from computer graphics and from prior research on WOS [2], RQMC yields modest but consistent improvements in root mean squared error and in variance decay. Empirically, we observe variance rates close to $n^{-1.2}$ in several settings, compared with the n^{-1} baseline of Monte Carlo which correspond to a gain in the order of 5-10x for the same sample size. We provide a theoretical analysis of the convergence rate, making use of results available in the literature regarding RQMC rates of convergence for discontinuous integrands [3]. We also report preliminary results on combining larger termination thresholds with Richardson extrapolation: when paired with RQMC, this strategy can achieve accuracy comparable to small-threshold runs while reducing average walk length and wall-clock time.

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Thursday June 11th – Afternoon/1, 16:30 – 17:00, JCMB Lecture Theatre C

Bayesian inference for output-feedback control of uncertain linear systems

Session: Bayesian inference using Monte Carlo and quasi-Monte Carlo methods p. 55

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This work presents a digital twin framework for output-feedback stabilization and parameter identification in uncertain dynamical systems. A digital model evolves in parallel with the physical process, assimilating measurement data in real time. Through observer design, the twin reconstructs the system state and generates stabilizing feedback, while model parameters are simultaneously inferred from data of the controlled dynamics using a Bayesian approach. Numerical results for the coupled physical-digital dynamics demonstrate how digital twins can act jointly as observers, estimators, and control agents, ensuring robust performance under uncertainty.

Thursday June 11th – Afternoon/1, 17:00 – 17:30, JCMB Lecture Theatre A

Optimal approximation of piecewise smooth functions from information contaminated with random noise

Session: Stochastic computation and complexity, Part 6 p. 54

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Approximation of piecewise smooth functions with unknown break points is a challenging task, especially when the available information about function values is contaminated with some noise. This problem was solved in [1] for the case of deterministic and bounded noise, where an algorithm was constructed achieving the optimal rate for L^p approximation ($1 \leq p \leq \infty$). In this talk, we extend the above results to the case of random (including Gaussian) noise, where for each individual function the error is defined as the q th moment ($1 \leq q < \infty$) of the L^p error with respect to the noise. In the case of 'small' noise the algorithm in [1] turns out to be optimal also for random noise, but for 'large' noise it suffers from overfitting. However, its modification consisting in appropriate oversampling already leads to optimal approximation. Moreover, the optimal rate is the same as for (globally) smooth functions [2].

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Thursday June 11th – Afternoon/1, 17:00 – 17:30, JCMB Lecture Theatre C

A Novel Convolutional Path Approach for Sampling with Interacting Particle Systems

Session: Bayesian inference using Monte Carlo and quasi-Monte Carlo methods p. 55

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Accurate and efficient Bayesian inference often requires sampling from high-dimensional, strongly non-Gaussian, and multimodal posterior distributions, posing significant challenges for existing particle-based methods. While kernel-based particle flows such as the Kernel Fisher–Rao (KFR) flow [1] provide flexible, gradient-free sampling strategies, they can suffer from poor multimodal coverage due to the limitations of geometric interpolation between prior and posterior distributions.

We develop a deterministic particle flow framework based on the convolutional path [2,3,4], a smoother and more gradual interpolation that is better suited for complex posterior landscapes. The convolutional path, commonly used in diffusion-based sampling, mitigates the mass “beaming” effect of geometric paths and is therefore particularly attractive for digital twin applications, where maintaining multiple competing hypotheses is essential.

We formulate the particle evolution as an interacting particle system governed by a velocity field derived from a Poisson equation associated with the convolutional path. To enable practical computation, we adopt a flexible Galerkin projection framework, generalizing existing kernel-based approaches and allowing the use of structured particle sets such as quasi-Monte Carlo points or sparse grids. Unlike classical KFR flows, the proposed approach incorporates gradient information of the prior and target models, trading gradient-free operation for improved robustness in multimodal settings.

The focus of this contribution is on the theoretical formulation, Monte Carlo approximations, and implementation strategy of the proposed flow. Ongoing work aims to analyze stability, computational cost, and effectiveness in representative digital twin scenarios involving multimodal uncertainty. This project highlights a promising direction for the development of particle flow methods for challenging Bayesian inference problems.

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Thursday June 11th – Afternoon/2, 15:30 – 16:00, JCMB 5326

Further investigations of the use of quasi-Monte Carlo in a Stochastic Optimal Control Framework for Maritime Mine Countermeasure Simulations

Session: Applications

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Modelling and simulating maritime 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 domain such that the residual MCM risk of encountering a mine after completion of the survey is below a certain user-defined threshold. In our previous work [1], we implemented the MCM problem as a stochastic optimal control problem where we considered a square search domain in which we suspect the presence of underwater sea mines. We modelled the residual risk constraint as an expected value integral for which we computed a solution by means of a quasi-Monte Carlo integration scheme (specifically a Rank-1 Lattice Rule). We combined the aforementioned integration scheme with a relaxation scheme for the optimization problem, and found a speed-up up to a factor 2 with respect to a standard Monte Carlo scheme. In subsequent work [2], we extended our implementation in order to accommodate multiple autonomous vehicles surveying the square search domain concurrently. Mathematically this is given as minimizing the total mission time needed to survey a designated domain Ω with a given Residual MCM Risk and a total of m individual vehicles, i.e.,

$$\min T_F, \quad (3)$$

subjected to

$$\mathbb{E}[q(T_F)] := \sum_{i=1}^m \int_{\Omega} e^{-\int_0^{T_F} \gamma(x_i(\tau), \omega) d\tau} f_X(\omega) d\omega \leq \text{Residual MCM Risk} \quad (4)$$

where the desired result consists of the positions of the different autonomous vehicle $x_i(t) := f(x(t), y(t), \psi(t), r(t))$, $\forall i \in \{0, \dots, m\}$ at times $t \in \{0, \dots, T_F\}$, i.e., the trajectories. We are currently extending our work such as to accommodate for the computation of trajectories in generalized convex polygons, e.g., pentagons, hexagons, heptagons. This is achieved by dividing our generalized convex polygon into a series of triangles, on which we use quasi-Monte Carlo points specifically designed for a triangular domain [3]. Furthermore, we investigate if the use of quasi-Monte Carlo points generated by means of Message Passing Monte Carlo (MPMC) [4], achieves a larger speed-up with respect to the Rank-1 Lattice rule, when combined with our relaxation scheme for the optimization problem.

Philippe Blondeel, P., Van Utterbeeck, F., Lauwens, B., “Application of quasi-monte carlo in mine countermeasure simulations with a stochastic optimal control framework” In

Proceedings of the 6th International Conference on Monte Carlo and Quasi-Monte Carlo Methods in Scientific Computing (MCQMC 2024) (To be published) (2026)

[2] Blondeel, P., Van Utterbeeck, F., Lauwens, B., “A stochastic optimal control formulation for mine counter measure simulations with multiple autonomous survey vehicles” In Proceedings of the 19th NATO ORA Conference 2025 (SAS-196) (To be published) (2026)

[3] K. Basu, and A. B. Owen, “Low Discrepancy Constructions in the Triangle”, SIAM Journal on Numerical Analysis, vol. 53, no. 2, pp 743-761, 2015

[4] K. Ruscha, N. Kirk, M. Bronstein, C. Lemieux, and D. Rus, “Message-Passing Monte Carlo: Generating low-discrepancy point sets via graph neural networks”, Proceedings of the National Academy of Sciences vol. 121, no. 40, 2024

Thursday June 11th – Afternoon/2, 15:30 – 16:00, JCMB 5327

Skew-symmetric schemes for robust SDE sampling.

Session: Sampling

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Coauthor(s): Yuga Iguchi, Samuel Livingstone, Nikolas Nusken and Rui-Yang Zhang.

We propose a new simple and explicit numerical scheme for time-homogeneous stochastic differential equations (SDEs), focusing on the case where the drift does not satisfy the Lipschitz property. The scheme is based on sampling increments at each time step from a skew-symmetric probability distribution, with the level of skewness determined by the drift and volatility of the underlying process. We show that as the step-size decreases the scheme converges weakly to the SDE of interest. We then consider the problem of simulating from the limiting distribution of an ergodic SDE using the numerical scheme with a fixed step-size. We establish conditions under which the numerical scheme converges to equilibrium at a geometric rate, and quantify the bias between the equilibrium distributions of the scheme and of the true diffusion process. Our results are supported via numerical simulations, which indicate that the schemes possess a robustness property with respect to different step-sizes.

[1] Y. Iguchi, S. Livingstone, N. Nusken, G. Vasdekis, R. Yang, Skew-symmetric schemes for stochastic differential equations with non-Lipschitz drift: an unadjusted Barker algorithm (2026+), Accepted at *IMA Journal of Numerical Analysis*.

Arxiv version: <https://arxiv.org/abs/2405.14373>

Thursday June 11th – Afternoon/2, 15:30 – 16:00, JCMB 5328

A Chen-Strichartz series expansion for Lévy models

Session: SDEs and Finance

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For deterministic differential equations and for continuous stochastic differential equations, the Chen-Strichartz series expansion, an expansion of the solution in terms of commutators of vector fields and iterated integrals, is well-known to play a central role in the development of numerical integration schemes that preserve qualitative properties of the solution. For stochastic differential equations that are driven by Lévy processes, the flow map, which describes the evolution of the solution, involves additional operators arising from jumps. We will derive a Chen-Strichartz series representation, depending only on commutators of vector fields and iterated integrals, and we will provide an explicit expression for the components in this series, generalising previous results for deterministic and continuous stochastic differential equations. We will illustrate the new Chen-Strichartz series representation in the application to a multi-dimensional stochastic volatility model.

Thursday June 11th – Afternoon/2, 16:00 – 16:30, JCMB 5326

Uncertainty Quantification in Stochastic Modelling of Proton Beam Therapy

Session: Applications

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Proton Beam Therapy (PBT) is a method for radiation-based cancer treatment. Due to the sharply peaked dose-depth curve characteristic of protons, and the fact that protons stop at a finite depth inside the tissue, PBT is especially useful when treating tumours situated close to vital organs, which need to be spared from radiation damage. In practice, uncertainties in inferred material properties induce uncertainties in the resulting stopping distance and dose-depth curve produced by the proton beam. If these uncertainties are too large, we no longer have enough confidence in the correct dose being deposited inside the tumour, rather than in surrounding vital organs.

In this talk, we introduce a stochastic differential equation model for proton dynamics in the therapeutic setting. Using model parameters as a proxy for uncertain material properties, we quantify the sensitivity of the model dose curve to these parameters. Specifically, we take a pathwise sensitivity approach to estimate the gradients of the dose distribution with respect to the parameters related directly to the dynamics of energy loss. We evaluate both the dose profile and its gradients with respect to model parameters using Monte Carlo simulation of the underlying augmented SDE system.

Thursday June 11th – Afternoon/2, 16:00 – 16:30, JCMB 5327

Diffusion-Guided Proposals for Efficient High-Dimensional MCMC

Session: Sampling

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We propose an MCMC algorithm that leverages a diffusion model as a nonlocal proposal mechanism. The method couples a forward diffusion with its time-reversed counterpart to generate structured, nonlocal moves guided by an estimated score function, and restores exactness through a Metropolis–Hastings correction. Unlike local proposals such as random-walk or Langevin updates, diffusion-guided moves traverse low-probability regions efficiently and facilitate transitions between separated modes. We analyze how the discretization step size and the diffusion time horizon influence acceptance and efficiency, deriving acceptance-rate expansions that quantify the effect of score approximation error. For high-dimensional product targets, we characterize scaling behavior and identify a trade-off between step size / diffusion horizon and acceptance probability, paralleling optimal-scaling results for existing MCMC methods. Experiments on multimodal targets demonstrate improved effective sample size per computational cost relative to classical local MCMC, while remaining robust under moderate score misspecification.

Thursday June 11th – Afternoon/2, 16:00 – 16:30, JCMB 5328

Numerical Methods for Singular SDEs

Session: SDEs and Finance

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Many applications, such as systems of interacting particles in physics, require the simulation of diffusion processes with singular coefficients. Standard Euler schemes are then not convergent, and theoretical guarantees in this situation are scarce. In this work we introduce a Lyapunov-tamed Euler scheme, for drift coefficients for which the weak derivative is dominated by a function that obeys a certain generic Lyapunov-type condition. The general result is applied to systems of mean-field particles with singular repulsive interaction in 1D, yielding an error bound with polynomial dependency in the number of particles. Furthermore, we discuss preliminary developments in the field of path-wise close approximations.

Thursday June 11th – Afternoon/2, 16:30 – 17:00, JCMB 5326

Uncertainty Quantification in Cloud Physics

Session: Applications

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The aim of the work is to quantify uncertainties associated to the most significant processes of the evolution of cirrus clouds, that is, clouds consisting of pure ice crystals. To this end, we consider a bulk scheme describing the processes of nucleation, i.e., the formation of clouds, growth of the ice crystals as well as sedimentation. As the process of nucleation leads to a stiff behavior of the corresponding differential equation, implicit and thus computationally expensive time integration methods are required.

Applying multilevel techniques for improving the efficiency of the Monte Carlo method, we face the difficulty that due to the high degree of the nonlinearity of the problem, discretizations on coarse grids are generally not sufficiently informative for an effective complexity reduction. We thus consider instead a combination with a multi-fidelity approach based on problem-adapted surrogate models.

The original model is formulated as a PDE. However, a description by an ODE serves as a simplification that facilitates the identification of effective strategies to combine promising surrogate models with the Multilevel Monte Carlo method. In this simplified setting, we have found a surrogate model based on a nonlinear parametrisation that effectively captures the characteristic behavior of the solutions to the differential equation in dependence of the observed uncertainties.

Thursday June 11th – Afternoon/2, 16:30 – 17:00, JCMB 5327

Metropolis-Hastings Acceptance Behavior for Bayesian Inversion with Random Forward Solvers

Session: Sampling

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In various application domains, one wishes to determine which parameter values should be used for a model to match its simulation output with measurement data. In practice however, measurement error on the data means that, at best, one can produce a so-called posterior probability distribution of these parameter values, given an assumed noise model. The Metropolis-Hastings is a straightforward approach that constructs a Markov chain with this posterior distribution as its invariant distribution. The parameter samples in the chain are selected through an accept-reject strategy, that accepts proposal samples, based on their likelihood, relative to that of the previous accepted sample.

Evaluating this likelihood requires the solution of the given model. Therefore, any errors in the discrete solver will result in errors in the likelihood evaluation. In this presentation, we discuss the case where Metropolis-Hastings is run on top of a stochastic solver, such as a Monte Carlo particle solver. In this case, the likelihood—and thus the acceptance probability—becomes a random variable whose variance scales with the number of random trajectories simulated by the solver [1]. We discuss the mismatch between theory and practice in this setting. To this end, we combine classical error analysis and simulation results to understand the behavior of the pseudomarginal Markov chains in this setting. We then present practical approaches for efficient estimation in such settings.

[1] Løvbak, E., Krumscheid, S., *An Investigation into the Distribution of Ratios of Particle Solver-based Likelihoods*. [arXiv:2508.05303](https://arxiv.org/abs/2508.05303) (2025).

Thursday June 11th – Afternoon/2, 16:30 – 17:00, JCMB 5328

Quantitative discrete time hedging under initial insider information

Session: SDEs and Finance

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The problem of quantitative discrete time hedging within the Black-Scholes model has been intensively studied for many years. In this presentation we study this problem under initial insider information. To include non-smooth terminal conditions, which induce a blow-up of trading strategies, we use adapted, i.e. not equidistant, deterministic time-nets. It is well known that the best possible rate of the L_2 -hedging error in the setting without insider information is $n^{-1/2}$, when the number n of trading dates tends to infinity.

We investigate the question to what extent this convergence improves in the presence of insider information. Moreover, we compute the limit of the re-scaled L_2 -hedging error. Because of the insider information, the underlying stochastic analysis in order to treat this models changes, for example Skorohod integration has to be used. Examples using parametrized Black-Scholes PDEs are given.

Thursday June 11th – Afternoon/2, 17:00 – 17:30, JCMB 5326

Integrated Monte Carlo Pipeline for Emulation and Inference in a Biomechanical Arterial Model

Session: Applications

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Patient-specific biomechanical models of stented and plaque-affected arteries can support intervention planning. We study an inference pipeline that uses Monte Carlo methods across emulation, sensitivity analysis and inverse optimisation. Direct simulation of high-cost biomechanical models limits rapid clinical inference. Therefore, statistical emulators (Gaussian processes, neural networks, and Bayesian splines), trained offline, can offer faster inference on new patient cases. Monte Carlo is used in emulator design and hyperparameter estimation. For inverse inference, Monte Carlo in Bayesian optimisation is used to recover biomechanical inputs from clinical observations using the emulator as a fast surrogate of the expensive forward model. This gives a practical route to parameter calibration when repeated simulator evaluations are prohibitive. For sensitivity analysis, we estimate Sobol indices via quasi-Monte Carlo to quantify the influence of inputs on model outputs. This is used to screen weak inputs, study identifiability in the inverse problem, and investigate identifiable parameter combinations. This talk links these stages into one applied workflow, demonstrating how Monte Carlo methods can be applied from emulator design and model fitting to sensitivity analysis and inverse optimisation within a clinically motivated arterial inference problem.

Thursday June 11th – Afternoon/2, 17:00 – 17:30, JCMB 5327

Adaptively Learning the Optimal Proposal for Self-Normalized Importance Sampling

Session: Sampling

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Estimating expectations under complex target distributions is central to machine learning and statistics. In applications such as Bayesian cross-validation and sensitivity analysis, direct sampling from the target can yield estimators with high or even infinite variance, making self-normalized importance sampling (SNIS) with a well-chosen proposal the standard remedy. Yet most existing proposals either approximate the target itself or target the proposal optimal for ordinary importance sampling rather than SNIS. We revisit the SNIS-optimal proposal of Hesterberg (1988), long overlooked because it is doubly intractable: the unknown expectation appears in its definition. We introduce a generic adaptive sampling framework that approximates this proposal by interleaving MCMC with running SNIS estimates, linking stochastic approximation, importance sampling, and MCMC. We prove a martingale central limit theorem for the resulting estimator, show that learning the proposal has no asymptotic cost, and establish a non-asymptotic contraction rate for the chi-squared divergence between the learned and optimal proposals. Experiments in Bayesian cross-validation validate the theory and show substantial variance reduction over existing alternatives.

Thursday June 11th – Afternoon/2, 17:00 – 17:30, JCMB 5328

Randomised Euler-Maruyama method for SDEs with Hölder continuous drift coefficient driven by α -stable Lévy process

Session: SDEs and Finance

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In this talk, we examine the performance of randomised Euler-Maruyama (EM) method for additive time-inhomogeneous SDEs with an irregular drift driven by symmetric α -stable process, $\alpha \in (1, 2)$. In particular, the drift is assumed to be β -Hölder continuous in time and bounded η -Hölder continuous in space with $\beta, \eta \in (0, 1]$. The strong order of convergence of the randomised EM in L^p -norm is shown to be $1/2 + (\beta \wedge (\eta/\alpha) \wedge (1/2)) - \varepsilon$ for an arbitrary $\varepsilon \in (0, 1/2)$, higher than the one of standard EM, which cannot exceed β . The result for the case of $\alpha \in (1, 2)$ extends the almost optimal order of convergence of randomised EM obtained in [2] for SDEs driven by Gaussian noise ($\alpha = 2$), and coincides with the performance of EM method in simulating time-homogeneous SDEs driven by α -stable process considered in [1].

[1] S. Biswas, C. Kumar, Neelima, G. dos Reis, C. Reisinger, *An explicit Milstein-type scheme for interacting particle systems and McKean–Vlasov SDEs with common noise and non-differentiable drift coefficients*, <https://arxiv.org/abs/2208.10052>.

[2] J. Bao, Y. Wu, *Randomised Euler-Maruyama method for SDEs with Hölder continuous drift coefficient: Randomised Euler-Maruyama method for SDEs with Hölder continuous drift coefficient*, BIT, 65(4), 2025.

Friday June 12th, 10:30 – 11:00, JCMB Lecture Theatre A

A construction for optimal least squares approximation

Session: Stochastic computation and complexity, Part 5

p. 56

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I will present an algorithm that generates points and weights for least squares approximation in a given basis. The error of the resulting weighted least squares algorithm has the same rate as best L_2 -approximation. The runtime of the construction is polynomial in the number of points if the basis is orthonormal in L_2 and bounded polynomially in the uniform norm. The presented result is from [3].

While the existence of sampling points with this property has been known before, the corresponding result was not constructive, as it relied on a non-constructive sparsification result of [1]. The key to the construction is a generalization of a sparsification result of [2] to a (potentially) infinite-dimensional setting.

[1] A. Marcus, D. Spielman and N. Srivastava, *Interlacing families II: Mixed characteristic polynomials and the Kadison-Singer problem*, Annals of Mathematics, 327–350, 2015.

[2] J. Batson, D. A. Spielman, and N. Srivastava, *Twice-Ramanujan Sparsifiers*, SIAM Review, 56, 315–334, 2014.

[3] A. Chkifa, M. Dolbeault, D. Krieg, and M. Ullrich, *Constructive discretization and approximation in reproducing kernel Hilbert spaces*, arXiv preprint, 2026. <https://arxiv.org/abs/2602.18719v1>

Friday June 12th, 10:30 – 11:00, JCMB Lecture Theatre B

Quasi-Monte Carlo for precision oncology – towards predictive digital twins

Session: MCQMC for digital twins

p. 56

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Quasi-Monte Carlo (QMC) methods have been successful for high dimensional integration, multivariate function approximation, density estimation, etc., in many application areas including uncertainty quantification problems driven by partial differential equations (PDEs) with random coefficients. This talk will showcase our latest work on the application of "lattice" QMC methods to a class of semi-linear parabolic reaction-diffusion PDEs used to model tumor growth and treatment. Mathematical models of tumor growth are largely phenomenological in nature, capturing infiltration of the tumor into surrounding healthy tissue, proliferation of the existing tumor, and patient response to therapies, such as chemotherapy and radiotherapy. Considerable inter-patient variability, inherent heterogeneity of the disease, sparse and noisy data collection, and model inadequacy all contribute to significant uncertainty in the model parameters. It is crucial that these uncertainties can be efficiently propagated through the model to compute quantities of interest (QoIs), which in turn may be used to inform clinical decisions. We will demonstrate both theoretically and computationally the success of QMC for this challenging nonlinear PDE problem.

Friday June 12th, 10:30 – 11:00, JCMB Lecture Theatre C

Multilevel double-loop quasi-Monte Carlo methods for nested integration

Session: Recent advances in hierarchical methods for uncertainty quantification, Part 2
p. 57

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In this talk, we present efficient estimators for nested integrals of the form $\int f \left(\int g(\mathbf{y}, \mathbf{x}) d\mathbf{x} \right) d\mathbf{y}$, where f is nonlinear. Such nested structures significantly increase the computational complexity of standard Monte Carlo (MC) estimators, from $\mathcal{O}(TOL^{-2})$ for single integrals to $\mathcal{O}(TOL^{-3})$ for a prescribed error tolerance $TOL > 0$. To address this challenge, we develop multilevel double-loop estimators based on quasi-Monte Carlo (QMC) and randomized QMC (rQMC) methods, which exploit integrand regularity to improve convergence rates. We investigate how different randomization strategies influence the overall computational cost and show how these methods can be combined with hierarchical discretizations, where both the number of inner function evaluations and the accuracy of finite element approximations of the inner integrand g define the levels. The resulting estimators achieve the same accuracy as standard MC methods at a computational cost below $\mathcal{O}(TOL^{-2})$. We demonstrate their performance in the context of expected information gain (EIG) for Bayesian optimal experimental design, where the outer integrand f is the logarithm, and the inner integrand g is the likelihood of data observations. To handle the resulting singular behavior of the logarithm near the boundaries of the integration domain, we introduce tailored techniques that improve integrand regularity and enhance the efficiency of QMC-based estimators.

Friday June 12th, 10:30 – 11:00, JCMB 5326

Multifidelity simulation and inference methods for non-Markovian reaction networks*Session: Monte Carlo Methods for Stochastic Reaction Networks* p. 58

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Stochastic models of biochemical reaction networks are widely used to capture intrinsic noise in cellular systems. The typical formulation of these models are based on Markov processes for which there is extensive research on efficient simulation and inference. However, there are biological processes, such as gene transcription and translation, that introduce history dependent dynamics requiring non-Markovian processes to accurately capture the stochastic dynamics of the system. This greater realism comes with additional computational challenges for simulation and inference. In this work, we develop efficient non-Markovian simulation algorithms for well-mixed stochastic biochemical reaction networks that include state and time-dependent delays. Our methods generalize the next reaction method and τ -leaping method to support arbitrary inter-event time distributions while preserving computational scalability. We also introduce a coupling scheme to generate exact non-Markovian sample paths that are correlated to an approximate non-Markovian τ -leaping sample path. This enables substantial computational gains for Bayesian inference of model parameters through multifidelity simulation-based inference schemes. We demonstrate the effectiveness of our approach on a gene regulation model with delayed autoinhibition, showing substantial gains in both simulation accuracy and inference efficiency of two orders of magnitude. These results extend the practical applicability of non-Markovian models in systems biology and beyond

Friday June 12th, 11:00 – 11:30, JCMB Lecture Theatre A

Function discretization and related questions*Session: Stochastic computation and complexity, Part 5* p. 56

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Coauthor(s): F. Bartel, L. Kämmerer, M. Schäfer, T. Ullrich

In this talk, based on the results from [1], we will investigate the problem of continuous norm discretization, construction of tight frames and exact Marcinkiewicz-Zygmund inequalities, and touch some related questions on the reconstruction of multivariate functions from their samples.

[1] Bartel F., Kämmerer L., Pozharska K., Schäfer M., Ullrich T. Exact discretization, tight frames and recovery via D -optimal designs. SMAI J. Comp. Math. 2025, **11**, 607–636.

Friday June 12th, 11:00 – 11:30, JCMB Lecture Theatre B

Efficient Entropy-Driven Strategies for Bayesian Optimal Experimental Design

Session: MCQMC for digital twins

p. 56

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Bayesian optimal experimental design (OED) seeks experimental configurations that maximize the expected informativeness of the resulting data, most commonly measured by the expected information gain. A key computational bottleneck in this setting is the evaluation of nested integrals required to compute this quantity. In this talk, we identify settings in which the differential entropy of the likelihood is either independent of the design or can be evaluated efficiently, allowing the expected information gain to be reformulated as a maximum entropy estimation problem. Building on this reformulation, we propose a computational approach that approximates the evidence density using Monte Carlo or quasi-Monte Carlo methods and evaluates differential entropy with only a modest number of additional likelihood evaluations. We provide a rigorous convergence analysis of the resulting estimators and show that they achieve favorable rates compared to existing approaches under mild smoothness assumptions. Numerical experiments on benchmark inverse problems demonstrate substantial computational savings without loss of accuracy.

Friday June 12th, 11:00 – 11:30, JCMB Lecture Theatre C

A function approximation algorithm using multilevel active subspaces

Session: Recent advances in hierarchical methods for uncertainty quantification, Part 2

p. 57

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The Active Subspace (AS) method is a widely used technique for identifying the most influential directions in high-dimensional input spaces that affect the output of a computational model. The standard AS algorithm [1] requires a sufficient number of gradient evaluations (samples) of the input output map to achieve quasi-optimal reconstruction of the active subspace, which can lead to a significant computational cost if the samples include numerical discretization errors which have to be kept sufficiently small. To address this issue, we propose a multilevel version of the AS method (MLAS) [2] that utilizes samples computed with different accuracies and yields different active subspaces across accuracy levels, which can match the accuracy of single-level AS with reduced computational cost, making it suitable for downstream tasks such as function approximation. In particular, we propose to perform the latter via optimally-weighted least-squares polynomial approximation in the different active subspaces, and we present

an adaptive algorithm to choose dynamically the dimensions of the active subspaces and polynomial spaces. We demonstrate the practical viability of the MLAS method with polynomial approximation through numerical experiments based on random partial differential equations (PDEs).

- [1] Constantine, Paul G. Active subspaces: Emerging ideas for dimension reduction in parameter studies. Society for Industrial and Applied Mathematics, 2015.
- [2] Nobile, Fabio, Matteo Raviola, and Raúl Tempone. "A function approximation algorithm using multilevel active subspaces." To appear in: Christiane Lemieux, Ben Feng (eds.), Monte Carlo and Quasi-Monte Carlo 2024: MCQMC 2024, Waterloo, Canada, August 18–23, Springer Proceedings in Mathematics & Statistics, Vol. 522, Springer, Cham, 2026.

Friday June 12th, 11:00 – 11:30, JCMB 5326

Effects of Model Reduction on Coherence and Information Transfer in Stochastic Biochemical Systems

Session: Monte Carlo Methods for Stochastic Reaction Networks

p. 58

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Simplified stochastic models are widely used in Monte Carlo-based analyses of biochemical reaction networks to study frequency-resolved noise propagation and information transmission. Key quantities of interest include coherence spectra and mutual information (MI) rates, which are often estimated from reduced models under assumptions of timescale separation. It is commonly presumed that such reductions preserve these information-theoretic measures of the underlying full systems. In this work, we demonstrate that this assumption can be violated in a systematic way. While reduced models typically reproduce low-order statistics of molecular copy numbers accurately, they can exhibit substantial errors in the coherence spectrum, particularly at intermediate and high frequencies. These spectral discrepancies directly translate into significant inaccuracies in MI rate estimates obtained from Monte Carlo simulations. We show that the origin of these errors lies in the interplay between reaction network structure, the chosen model reduction strategy, and the asymptotic limits used to relate full and reduced descriptions. Using canonical models of enzyme catalysis and gene expression, we illustrate how commonly employed reductions can distort frequency-dependent noise propagation and information flow. Our results highlight important limitations of simplified stochastic models and have direct implications for the reliable use of Monte Carlo methods in quantifying information transmission in stochastic reaction networks.

Friday June 12th, 11:30 – 12:00, JCMB Lecture Theatre A

Precise asymptotics and exact expressions for QMC-errors of Fibonacci lattices

Session: Stochastic computation and complexity, Part 5

p. 56

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The quasi-Monte Carlo method (QMC) for approximating the integral of a function via the mean of a set of sample points has been studied for a long time and analyzing its performance is a classical problem in numerical analysis. Here we will focus on determining good point sets over the torus where the worst-case error is measured with respect to a Sobolev-Hilbert space of dominating mixed smoothness. Kernel methods allow for an easy determination of the worst-case error and serve as a starting point for our analysis.

While optimal point sets in an asymptotic sense are well-established by now, in certain situations numerical computations [1] and partial results [2, 3] suggest that one can even determine the globally optimal point sets. In the two-dimensional torus so-called Fibonacci lattices frequently show up in this context. This talk gives an overview of known results in this direction as well as recent developments on the precise asymptotics for these special point sets. The involved techniques combine classical analysis with number theoretic methods.

Rather surprisingly, in the case of integer smoothness we even observe simple closed-form expressions for these worst-case errors, suggesting that the problem of optimal QMC-points is exactly solvable in this sense.

[1] A. Hinrichs and J. Oettershagen, Optimal point sets for quasi-Monte Carlo integration of bivariate periodic functions with bounded mixed derivatives, in *Monte Carlo and quasi-Monte Carlo methods*, 385–405, Springer Proc. Math. Stat., 163, Springer, ; MR3536671

[2] D. Bilyk, N. Nagel, I. Ruohoniemi, Minimizing point configurations for tensor product energies on the torus, *arXiv:2510.25442* (2025)

[3] N. Nagel, Global optimality of 3- and 5-point Fibonacci lattices for quasi-Monte Carlo integration and general energies, *J. Complexity* **93** (2026), Paper No. 102012, 15 pp.; MR4998755

Friday June 12th, 11:30 – 12:00, JCMB Lecture Theatre B

A one-shot method for Bayesian optimal experimental design

Session: MCQMC for digital twins

p. 56

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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.

Friday June 12th, 11:30 – 12:00, JCMB Lecture Theatre C

Multilevel Gaussian Processes with Applications to Inverse Problems

Session: Recent advances in hierarchical methods for uncertainty quantification, Part 2
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In this talk, we present a multilevel Gaussian process (GP) regression framework for approximating response surfaces arising from parametrized partial differential equations. By modelling level increments independently with Matérn-kernel GPs and allocating samples flexibly across discretization levels, the multilevel approach achieves substantial computational savings over standard single-level GP regression. We derive L^2 convergence rates for the posterior mean and variance, incorporating maximum likelihood estimation of the marginal variance and accounting for kernel misspecification. When the regularity of the level increments or the cost of the numerical solver is not known a priori, we propose an adaptive algorithm based on sequential design with cost-adapted active learning criteria for optimal sample allocation across levels. The theoretical rates are confirmed by numerical experiments. Finally, we apply the multilevel GP surrogate to Bayesian inverse problems and establish Hellinger distance bounds between the true and approximate posterior.

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[2] T. Karvonen, G. Wynne, F. Tronarp, C. Oates, S. Särkkä, *Maximum Likelihood Estimation and Uncertainty Quantification for Gaussian Process Approximation of Deterministic Functions*, SIAM/ASA Journal on Uncertainty Quantification, 8(3), 2020, 926–958.

[3] A. M. Stuart, A. L. Teckentrup, *Posterior Consistency for Gaussian Process Approximations of Bayesian Posterior Distributions*, Mathematics of Computation, 87(310), 2017, 721–753.

Friday June 12th, 11:30 – 12:00, JCMB 5326

Tensor Train Decomposition for Optimal Importance Sampling in Stochastic Reaction Networks

Session: Monte Carlo Methods for Stochastic Reaction Networks
p. 58

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We consider the problem of estimating rare event probabilities for stochastic reaction networks, which is challenging for Monte Carlo (MC) methods due to high relative variance. We use the importance sampling (IS) technique to reduce the variance of the MC estimator. Finding the optimal IS parameters leads to a stochastic optimal control problem, which is prone to the curse of dimensionality and is infeasible to solve for high-dimensional systems. In this work, we explore a low-rank tensor train approximation to estimate the optimal IS parameters. The tensor train method provides a flexible approximation of the IS parameters, significantly reducing the variance with little additional computational cost. The main advantage of our approach is that the tensor approximation error does not introduce a bias in the quantity of interest but only affects the variance of the IS estimator. Our numerical results show a substantial reduction in computational cost compared to the standard MC method when estimating the probabilities of rare events.

Friday June 12th, 12:00 – 12:30, JCMB Lecture Theatre A

Regularizing the randomized QMC quadratures via the Median of Means.

Session: Stochastic computation and complexity, Part 5

p. 56

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Let $(Q_n)_n$ be a sequence of independently randomized quasi Monte Carlo quadratures. In many cases (e.g. Q_n being shifted rank-1 lattice rules, Latin hypercube samplings or quadratures based on scrambled $(0, m, s)$ -nets) it turns out that for each $p \in [1, 2)$ there are functions $f_p \in L^p$ for which $(Q_n f_p)_n$ does not converge almost surely to the integral of f_p . To get rid of this problem we propose to use the median-of-means estimators

$$Q_{n,k}f = \text{med}\{Q_n^{(1)}f, \dots, Q_n^{(k)}f\},$$

where $Q_n^{(j)}$ are independent copies of Q_n .

In the first part of the talk we provide a criterion allowing to deduce the non-convergence results and show how it relates to the most widely-used randomized QMC quadratures.

In the second part of the talk we discuss the convergence of $(Q_{n,k(n)}f)_n$, in particular showing that for $k(n) = \Omega(\log(n))$ we have the almost sure convergence to the integral and upper-bounding the speed of convergence. Furthermore, under some mild additional conditions we compare the L^2 convergence rates of $(Q_n f)_n$ and $(Q_{n,k} f)_n$.

Friday June 12th, 12:00 – 12:30, JCMB Lecture Theatre B

From Flat to Curved: UQ for PDEs on Random Surfaces using QMC

Session: MCQMC for digital twins

p. 56

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The modelling of processes governed by partial differential equations (PDEs) posed on random domains arises in a wide range of applications, including biology, medical imaging, and engineering. In this work, we investigate uncertainty quantification for PDEs subject to domain uncertainty by numerically approximating the expectation of the PDE solution using randomly shifted lattice quasi-Monte Carlo (QMC) cubature rules.

Based on our previous work in [1], we consider a reference configuration that is not a Euclidean domain but rather a \mathcal{C}^2 -hypersurface, thereby incorporating curvature and other geometric features into the problem. We address this question under the additional assumption that the domain mapping is governed by a random field obtained by composing Gevrey functions with smooth transformations of random variables. This leads to domain mappings belonging to a generalized Gevrey class, in which the parametric derivatives of the perturbation field satisfy a more intricate regularity bound.

As a model problem, we consider the Laplace–Beltrami equation. The theoretical findings are supported by numerical experiments.

- [1] Djurdjevac, Ana, Kaarnioja, Vesa, Schillings, Claudia, & Zepernick, André-Alexander (2025). Uncertainty quantification for stationary and time-dependent PDEs subject to Gevrey regular random domain deformations. Preprint, *arXiv:2502.12345 [math.NA]*.

Friday June 12th, 12:00 – 12:30, JCMB Lecture Theatre C

Level-set approximation of noisy functions

Session: Recent advances in hierarchical methods for uncertainty quantification, Part 2

p. 57

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In this talk, we consider the problem of numerically approximating the level set of a noisy multivariate function which is only accessible via pointwise sampling. A key application is the estimation of failure probability regions: given a random PDE that depends on a set of deterministic parameters and a failure criterion, determine the parameter region where the probability of failure exceeds a given safety threshold.

We present a level-set estimation algorithm for Lipschitz-continuous functions which is adaptive in terms of both parameter-space approximation and sampling, and automatically increases accuracy close to the level set. This algorithm is compatible with general Monte Carlo estimators and achieves improved cost complexity rates with respect to non-adaptive approximations. We provide numerical experiments based on random PDEs and computer vision in support of our theoretical findings.

- [1] M. Croci, A.-L. Haji-Ali, and I. C. J. Powell. *An adaptive sampling algorithm for level-set approximation*. Preprint. <https://arxiv.org/abs/2509.14896> . (2025).

Friday June 12th, 10:30 – 11:00, JCMB 5327

A Bayesian Approach to Low Discrepancy Subset Selection

Session: Bayesian methods

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Low-discrepancy designs play a central role in quasi-Monte Carlo methods and are increasingly influential in other domains. In recent years, one such low-discrepancy construction method called subset selection has received a lot of attention. Given a large population, one optimally selects a small low-discrepancy subset with respect to a discrepancy-based objective. In this talk, we establish, that the subset selection problem with respect to kernel discrepancies is NP-hard. Motivated by this intractability, we propose a Bayesian Optimisation procedure for the subset selection problem utilising the recent notion of deep embedding kernels. We demonstrate the performance of the BO algorithm to minimise discrepancy measures and note that the framework is broadly applicable any design criteria.

Friday June 12th, 10:30 – 11:00, JCMB 5328

Uniform Distribution in the p -adic Integers and Applications

Session: Point sets

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While uniform distribution theory in the real setting is typically formulated for sequences in the unit interval $[0, 1]$, its p -adic analogue concerns sequences in the ring of p -adic integers \mathbb{Z}_p (for a prime p). The classical example of a low-discrepancy sequence in \mathbb{Z}_p is the p -adic analogue of the real Kronecker sequence, namely $(x_n) = an + b$ with $a \in \mathbb{Z}_p^\times$ and $b \in \mathbb{Z}_p$. For a long time, this simple construction was essentially the only explicit example known. Only recently has a more general construction, based on permutation polynomial sequences, been discovered.

In this talk, we investigate whether and to what extent this construction can be generalized to 1-Lipschitz maps, both in the one-dimensional and the multi-dimensional setting. Among other results, we show that the Hausdorff dimension of orbit closures of affine maps in \mathbb{Z}_p^d is always equal to 1. This implies, in particular, that dense multi-dimensional Kronecker sequences do not exist in the p -adic setting. We also demonstrate that the connection between discrepancy theory and the pair correlation statistic admits a particularly clear description over \mathbb{Z}_p .

Finally, we discuss how our results influence the classical real setting via the Monna map. Building on earlier work, this map allows one to transfer information from the p -adic framework to the real unit interval $[0, 1]$.

Friday June 12th, 10:30 – 11:00, JCMB 6206

Asymptotic error bounds for numerical integration of infinite-variate functions in tensor product RKHS

Session: Approximation

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We analyze the n -th minimal worst-case error e_n of deterministic algorithms for numerical integration of infinite-variate functions. The underlying function space is an RKHS defined by a countable tensor product of univariate kernels. Known results from [1] and [2] regarding the decay $\alpha > 0$ of e_n establish upper bounds of the form $n^{-\alpha+\varepsilon}$ for every $\varepsilon > 0$ and lower bounds of the form $n^{-\alpha}$. Building on this, we prove asymptotic upper and lower bounds of the form $n^{-\alpha}\psi(n)$ and provide explicit estimates for the sub-polynomial factor ψ . Finally, we demonstrate that these rates are achieved by the Multidimensional Decomposition Method (MDM) and present numerical results following [3].

- [1] L. Plaskota and G.W. Wasilkowski. “Tractability of infinite-dimensional integration in the worst case and randomized settings”. *Journal of Complexity* 27.6 (2011)
- [2] M. Gnewuch, M. Hefter, A. Hinrichs, and K. Ritter. “Embeddings of weighted Hilbert spaces and applications to multivariate and infinite-dimensional integration”. *Journal of Approximation Theory* (2017).
- [3] A. D. Gilbert, F. Y. Kuo, D. Nuyens, and G. W. Wasilkowski. “Efficient Implementations of the Multivariate Decomposition Method for Approximating Infinite-Variate Integrals”. *SIAM Journal on Scientific Computing* 40.5 (2018)

Friday June 12th, 11:00 – 11:30, JCMB 5327

Markov category Monte Carlo: a categorical account of Metropolis–Hastings

Session: Bayesian methods

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Traditionally, probability and statistics have been founded on measure theory. However, for researchers in applied probability, statistics and machine learning, it is very rare that one actually refers to explicitly-constructed probability spaces, sigma-algebras or measurability. The recent perspective of categorical probability [2,4] instead begins with compositional structure, and provides a rigorous approach to reason about stochasticity, with measure-theoretic probability being an example, rather than the foundation. In this talk, I will give an account of Metropolis–Hastings (MH) in the categorical setting of CD categories [3]. Building on a recently-proposed involutive perspective on MH [1], this will culminate in a set of extremely general necessary and sufficient conditions for generalised-MH-type algorithms to be reversible. This proof is purely categorical, making no explicit reference to kernels, measures or sigma-algebras, and is proven pictorially using string diagrams. The previously-established sufficient conditions for reversibility can be recovered by instantiating our general result in a particular category of Markov kernels. In my talk, I will not assume any prior knowledge of category theory.

[1] Andrieu, C., Lee, A., Livingstone, S. (2020). A general perspective on the Metropolis-Hastings kernel. <http://arxiv.org/abs/2012.14881>.

[2] Cho, K., Jacobs, B. (2019). Disintegration and Bayesian inversion via string diagrams. *Mathematical Structures in Computer Science*, 29(7), 938–971.

[3] Cornish, R., Wang, A.Q., 2026. A categorical account of the Metropolis-Hastings algorithm. <https://arxiv.org/abs/2601.22911>.

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Friday June 12th, 11:00 – 11:30, JCMB 5328

On choosing parameters for Kronecker sequences

Session: Point sets
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Kronecker sequences are closely related to rank-1 lattices but have not been studied or used quite as extensively as the latter. Improvements to their associated error bounds were obtained by Dick et al. (2018) [1] using Besov spaces, which allows the smoothness of integrands to be captured in the convergence rate of those bounds. In this talk, we explore a few different approaches for using Kronecker sequences. One is to try to find vectors of good irrational numbers to construct the sequences. Here we review existing approaches and propose some new ones. The other is to randomly choose the vector of irrational numbers, and then study whether taking the median of the replicates can lead to better results than taking the average. We do so by establishing a bound on the tail probability of the error for the median-based estimator in the case of Kronecker sequences, similarly to what has been recently done by other authors for rank-1 lattices,

digital nets and polynomial lattice rules. We also present numerical results comparing different constructions and estimators.

[1] J. Dick, F. Pillichshammer, K. Suzuki, M. Ullrich, and T. Yoshiki. Lattice-based integration algorithms: Kronecker sequences and rank-1 lattices. *Annali di Matematica*, 197:109–126, 2018.

Friday June 12th, 11:00 – 11:30, JCMB 6206

Learning Anisotropy Parameters to Improve ANOVA Approximations

Session: Approximation

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This talk is concerned with learning the anisotropic smoothness of a function based on scattered data. We use this smoothness information in our approximation algorithm improving the convergence rate. In particular, we use the least squares approximation with trigonometric polynomials and frequency boxes with optimized side ratio. Here the NFFT (Nonequispaced Fast Fourier Transform) is applicable to accelerate the computation time of the approximation. We combine these findings with the truncated ANOVA (analysis of variances) decomposition. This method makes high-dimensional problems feasible. The optimal choice of frequency boxes from above occurs here multiple times for every ANOVA term. With our approach we are able to optimize hundreds of parameters in order to gain approximation accuracy with minimal overhead. Numerical experiments indicate the applicability of our results. This talk based on a joint work with Felix Bartel.

[1] **F. Bartel and P. Schröter**. Learning and Leveraging Anisotropy Parameters in ANOVA Approximation. *J. Fourier Anal. Appl.*, 2026.

Friday June 12th, 11:30 – 12:00, JCMB 5327

MCMC for Bayesian inference of the non-conducting region in intra-atrial reentrant tachycardia

Session: Bayesian methods

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Cardiac arrhythmia arise from abnormal electrical activity in the heart and are associated with a large number of deaths. The underlying disease condition varies between individuals, necessitating patient-specific treatment. In this context, cardiac digital twins offer a promising new approach. However, current imaging techniques limit the fidelity with which individual cardiac anatomy and function can be modelled, making uncertainty quantification (UQ) during model calibration essential.

We employ Bayesian inference for parameter estimation in a cardiac electrophysiology model to perform UQ that accounts for measurement and discretization errors. In a two-dimensional cardiac tissue slab, we simulate the electrical signal propagation that coordinates heart contraction during a common arrhythmia, intra-atrial reentrant tachycardia. From mapping catheter data, we aim to estimate a geometrical parameter describing an electrically non-conducting region, or scar, which is directly linked to the occurring arrhythmia.

In our talk, we propose a Markov chain Monte Carlo method that requires a minimal number of samples for posterior estimation by defining a likelihood based on characterizing quantities of the data and by using an adaptive proposal distribution. To account for the discretisation error, we inflate the likelihood variance, and we tailor the meshing strategies used for the forward simulations in the accept-reject step. We illustrate the benefits of stochastic fits over deterministic fits with several examples.

Friday June 12th, 11:30 – 12:00, JCMB 5328

Stationary MMD Points

Session: Point sets

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Approximation of a target probability distribution using a finite set of points is a problem of fundamental importance in numerical integration. Several authors have proposed to select points by minimising a maximum mean discrepancy (MMD), but the non-convexity of this objective typically precludes global minimisation. Instead, we consider the concept of *stationary points of the MMD* which, in contrast to points globally minimising the MMD, can be accurately computed. Our main contributions are two-fold and theoretical in nature. We first prove the (perhaps surprising) result that, for integrands in the associated reproducing kernel Hilbert space, the numerical integration error of stationary MMD points vanishes *faster* than the MMD. Motivated by this *super-convergence* property, we consider MMD gradient flows as a practical strategy for computing stationary points of the MMD. We then prove that MMD gradient flow can indeed compute stationary MMD points, based on a refined convergence analysis that establishes a novel non-asymptotic finite-particle error bound.

Friday June 12th, 11:30 – 12:00, JCMB 6206

Optimal Sampling for Kernel Quadrature on Unbounded Domains

Session: Approximation

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Kernel quadrature is a widely used approach for approximating integrals of smooth functions, with the worst-case integration error commonly expected to decay at the minimax rate $n^{-\alpha/d}$ for functions of smoothness α in dimension d . Existing rate-optimal results typically rely on deterministic point sets tailored to a specific kernel, which makes them sensitive to kernel misspecification and limits their robustness in practice. In this work, we study randomized point-evaluation quadrature methods and focus on robustness rather than kernel-specific optimality. We construct an explicit, n -dependent sampling distribution that achieves the minimax optimal convergence rate $n^{-\alpha/d}$ for worst-case integration error over smoothness classes, without requiring knowledge of the underlying kernel. This kernel-agnostic design ensures robustness to misspecification while retaining rate-optimal performance. Our analysis covers unbounded sampling measures, including Gaussian distributions, going beyond the standard setting of compact domains. The results provide both a theoretical guarantee and a practical recipe for designing robust, rate-optimal randomized quadrature schemes.

[1] Hennig, P., Osborne, M. A., and Girolami, M. Probabilistic Numerics: Computation as Machine Learning. Cambridge University Press, 2022.

[2] Briol, F.-X., Oates, C. J., Cockayne, J., Chen, W. Y., and Girolami, M. On the Sampling Problem for Kernel Quadrature. In Proceedings of the 34th International Conference on Machine Learning, 2017.

[3] Briol, F.-X., Oates, C. J., Girolami, M., Osborne, M. A., and Sejdinovic, D. Probabilistic Integration: A Role in Statistical Computation? Statistical Science, 2019.

Friday June 12th, 12:00 – 12:30, JCMB 5328

A trapezoidal quadrature scheme for fractional Brownian motion

Session: Point sets

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We introduce an accurate and efficient approximation of the fractional Brownian motion (fBm) with Hurst parameter $H \in (0, \frac{1}{2}) \cup (\frac{1}{2}, 1)$ based on a variable-transformed trapezoidal quadrature of its infinite-dimensional Ornstein–Uhlenbeck representation. The resulting approximation allows one to use the Kalman filter for systems where the signal is driven by an fBm, a system which is non-Markovian and computationally difficult.

Friday June 12th, 12:00 – 12:30, JCMB 6206

Space-filling designs in the unit ball of a Reproducing Kernel Hilbert Space

Session: Approximation

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A Reproducing Kernel Hilbert Space (RKHS) is a functional Hilbert space where point evaluation is a continuous linear function. This is equivalent to the existence of a symmetric, positive semi-definite kernel by which it is fully characterized (see [3]). RKHSs have been extensively used in Machine Learning and statistics. We focus on the generalization of the notion of space-filling designs to these spaces.

The literature on surrogate modelling and optimal sampling techniques over sets of functions is scarce and mainly consists in dimensional reduction approaches, projecting the variables over finite dimensional spaces. Inevitably, these methods lead to a loss of information, as the functions will now be approximated by their projection. To side-step this issue, covariance kernels for Gaussian Processes Regression can be defined over the whole functional space. However, doing so requires training the models over experimental designs that have not been truncated a priori.

To overcome these limitations, we consider the Morris criterion, a generalization of the Minimax criterion (see [2]) proposed in [1], and adapt it to functional spaces. We focus on subsets in which the functional norm can be controlled, in particular, the unit ball of a RKHS. This leads to the definition of a constrained optimization problem with functional variables. We propose two algorithms for its resolution.

The first method leverages Moore-Aronszajn's Theorem (see [3]), which expresses any RKHS function as a potentially infinite linear combination of kernel evaluations. This allows us to define a relaxation of the problem, in which the evaluation centers and coefficients are treated as optimization variables. This approach enriches the functional basis at every step, ensuring functions are optimally spread over the domain without restricting them to a fixed finite-dimensional subspace.

The second method is based on an analytical approach, deriving necessary and sufficient conditions for optimality. These are then incorporated into the Simplex of Functions - One Shot Algorithm (SOFUN-OSA), a computationally efficient algorithm that guarantees optimality. Our numerical experiments show that both methods outperform truncated Karhunen-Loève dimension reduction in terms of minimal intra-pair distance and D-Optimality (see [1]).

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- [2] Pronzato, Luc, and Werner G. Müller. "Design of computer experiments: space filling and beyond." *Statistics and Computing* 22.3 (2012): 681-701.
- [3] Saitoh, Saburo, and Yoshihiro Sawano. *Theory of reproducing kernels and applications*. Vol. 44. Singapore: Springer Singapore, 2016.

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