Welcome to MCQMC 2022

We are delighted to welcome you to Linz for the *15th International Conference on Monte Carlo and Quasi-Monte Carlo Methods in Scientific Computing.* The MCQMC conference series is, together with its sister conference series, the conferences on Monte Carlo Methods (MCM), a major event for researchers in the Monte Carlo and quasi-Monte Carlo community. We are glad to host MCQMC in Austria for the second time.

As of July 7, MCQMC 2022 features 192 talks, among them nine plenary talks and two tutorials, and 28 special sessions. The speakers come from a variety of scientific backgrounds, countries, institutions and stages of their career. We hope that, after two long years with hardly any offline meetings, you will again have the opportunity to meet colleagues, establish new contacts, and get new ideas from this meeting by talking with your fellow participants. If so, this conference will have been a success.

We are aware that organizing MCQMC 2022 as one of the first on-site events after the pandemic has been a certain risk, and that some of the participants would have preferred an online or hybrid event for various reasons. Nevertheless, we are convinced that personal meetings with colleagues are essential for progress in science and for fruitful collaborations, which is why the organizing team of MCQMC 2022 has made this decision.

Located on the river Danube, about halfway between Salzburg and Vienna, Linz is the third-largest city in Austria, and a vibrant place that offers an interesting mix of architecture, culture, technology, and nature. We invite you to explore and enjoy summer in Linz.

We wish you a pleasant, productive, and interesting stay at MCQMC 2022!

Aicke Hinrichs, Peter Kritzer, and Friedrich Pillichshammer
MCQMC 2022 Conference Organizers

Johannes Kepler University (JKU) Linz and
RICAM, Austrian Academy of Sciences.

Conference website: `https://www.ricam.oeaw.ac.at/events/conferences/mcqmc2022/`
Conference email: `mcqmc2022@ricam.oeaw.ac.at`

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History

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

The conference was initiated by Harald Niederreiter, who co-chaired the first seven conferences of the series. From 2006 onwards, the 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. Montreal, 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).

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Special Thanks

The conference organizers would like to thank all sponsors for making this event possible. We also want to express our gratitude towards Professor Gerhard Larcher (Head of the Department of Financial Mathematics and Applied Number Theory at JKU Linz) and Professor Ronny Ramlau (Head of RICAM at the Austrian Academy of Sciences) for their support to host this conference at our institutions.

We are also very grateful to many colleagues at JKU Linz and the Austrian Academy of Sciences for their help and support during various planning stages of the conference, including Gabi Danter, Simon Eder, Renata Fleischner, Manuel Forster, Wolfgang Forsthuber, Louisa Hofmann, Johannes Thuswaldner, Florian Tischler, Melanie Traxler, Sandra Winzer, and Sarah Wolfsegger.

We wish to extend our thanks to the entire Steering Committee and Program Committee, and past MCQMC conference organizers for their contribution and support. We also thank our plenary speakers, tutorial speakers, special session organizers, and all session chairs for their help and support with the scientific organisation of the conference.

Last but not least, we are extremely grateful to many friends in the MCQMC community who helped us in various ways to organize MCQMC 2022, in particular Mike Giles, Takashi Goda, Fred J. Hickernell, Frances Y. Kuo, Christiane Lemieux, and Art B. Owen.

Schedule

Sunday, July 17, 2022 – Afternoon

13:30 – 16:00	Registration – Hall B (outside Lecture Hall 1)
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15:45 – 16:00	Coffee break
16:00 – 17:30	Lecture Hall 1 **Tutorial** ***Chris J. Oates*** **Sampling with Stein Discrepancies** p. 35 Chair: *Fred J. Hickernell*

Monday, July 18, 2022 – Morning I

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	Lecture Hall 1 **Technical Session** Chair: *Andreas Neuenkirch*	Lecture Hall 3 **Technical Session** Chair: *Bence Borda*	Lecture Hall 4 **Technical Session** Chair: *Ajay Jasra*	Lecture Hall 5 **Technical Session** Chair: *Elisabeth Ullmann*	Lecture Hall 6 **Technical Session** Chair: *Winfried Sickel*
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14:30 – 15:00	*Pieter Vanmechelen* Multilevel Markov Chain Monte Carlo for full-field data assimilation p. 221	*Markus Passenbrunner* Extremal distributions of discrepancy functions p. 168	*Régis Santet* Ensuring unbiased sampling of HMC schemes for non separable Hamiltonian systems p. 191	*Azar Louzi* A multilevel stochastic approximation algorithm for unbiased value-at-risk and expected shortfall estimation p. 151	*Leszek Plaskota* Adaptive methods for numerical approximation: an asymptotic analysis p. 172
15:00 – 15:30	Coffee break – Halls B and C				
15:30 – 16:30	Lecture Hall 1 **Plenary Talk** ***Michael Feischl*** **A quasi-Monte Carlo data compression algorithm for machine learning** p. 40 Chair: *Josef Dick*				
16:30 – 16:45	Conference Photo				
19:00 –	Conference Dinner – “Stadtliebe”, Landstraße 31, Linz				

Thursday, July 21, 2022 – Morning I

09:00 – 10:00	Lecture Hall 1 **Plenary Talk** ***Erich Novak*** **Optimal algorithms for numerical integration: recent results and open problems** p. 44 Chair: *Aicke Hinrichs*
10:00 – 10:30	Coffee break – Halls B and C

Thursday, July 21, 2022 – Morning II

	Lecture Hall 1 **Special Session** *Larisa Yaroslavtseva* Stochastic Computation and Complexity: Approximation of SDEs with Non-standard Coefficients, Part 2 of 2 p. 77 Chair: *Larisa Yaroslavtseva*	Lecture Hall 3 **Special Session** *David Krieg* and *Mario Ullrich* Approximation from Random Data, Part 1 of 2 p. 54 Chair: *David Krieg*	Lecture Hall 4 **Special Session** *Neil K. Chada* and *Simon Weissmann* Advanced Particle Methods for Bayesian Inference p. 50 Chair: *Neil K. Chada*	Lecture Hall 5 **Special Session** *Chiheb Ben Hammouda* and *Raúl Tempone* Monte Carlo Methods and Variance Reduction Techniques for Forward and Inverse Problems for Stochastic Reaction Networks p. 62 Chair: *Chiheb Ben Hammouda*	Lecture Hall 6 **Special Session** *Art B. Owen* and *Takashi Goda* Quasi-Monte Carlo Methods of High Order and Beyond, Part 1 of 2 p. 68 Chair: *Art B. Owen*
10:30 – 11:00	*Michaela Szölgyenyi* Existence, uniqueness, and approximation for jump-driven SDEs with discontinuous drift p. 213	*Mario Ullrich* On the power of function values for L_2-approximation p. 217	*Gottfried Hastermann* Analysis of a localized non-linear ensemble Kalman–Bucy filter with sparse observations p. 128	*Muruhan Rathinam* State and parameter estimation from partial state observations in stochastic reaction networks p. 178	*Josef Dick* Quasi-Monte Carlo methods for stochastic Landau-Lifshitz-Gilbert equations p. 106
11:00 – 11:30	*Chengcheng Ling* Taming singular SDEs: A numerical method p. 147	*Felix Bartel* Constructive subsampling of finite frames with applications in optimal function recovery p. 86	*Sahani Pathiraja* Theoretical insights on a class of control based particle filters and their approximations p. 169	*Zhou Fang* Stochastic filtering for multiscale stochastic reaction networks based on hybrid approximations p. 113	*Takashi Goda* Construction-free median lattice rules p. 122

Thursday, July 21, 2022 – Morning III

	Lecture Hall 1	Lecture Hall 3	Lecture Hall 4	Lecture Hall 5	Lecture Hall 6
	Special Session *Larisa Yaroslavtseva* Stochastic Computation and Complexity: Approximation of SDEs with Non-standard Coefficients, Part 2 of 2 p. 77 Chair: *Larisa Yaroslavtseva*	**Special Session** *David Krieg* and *Mario Ullrich* Approximation from Random Data, Part 1 of 2 p. 54 Chair: *David Krieg*	**Special Session** *Neil K. Chada* and *Simon Weissmann* Advanced Particle Methods for Bayesian Inference p. 50 Chair: *Neil K. Chada*	**Special Session** *Chiheb Ben Hammouda* and *Raúl Tempone* Monte Carlo Methods and Variance Reduction Techniques for Forward and Inverse Problems for Stochastic Reaction Networks p. 62 Chair: *Chiheb Ben Hammouda*	**Special Session** *Art B. Owen* and *Takashi Goda* Quasi-Monte Carlo Methods of High Order and Beyond, Part 1 of 2 p. 68 Chair: *Art B. Owen*
11:30 – 12:00	*Paweł Przybyłowicz* Strong and weak approximation of solutions of SDEs under noisy information about coefficients and driving Wiener process p. 175	*Matthieu Dolbeault* Weighted least-squares approximation in expected L^2 norm p. 109	*Tim Roith* A kernelized consensus-based optimization method p. 187	*Sophia Wiechert* Efficient importance sampling via stochastic optimal control for stochastic reaction networks p. 228	*Yoshihito Kazashi* Density estimation in RKHS with application to Korobov spaces in high dimensions p. 137
12:00 – 12:30	*Kathrin Spendier* Convergence of the tamed Euler–Maruyama method for SDEs with discontinuous and polynomially growing drift p. 203	*Joscha Prochno* Operator norms of random matrices with structured variance profile p. 174	*Björn Sprungk* Dimension-independent Markov chain Monte Carlo on the sphere p. 205		*Marcello Longo* Rate-optimality of an adaptive quasi-Monte Carlo finite element method p. 151
12:30 – 14:00	Lunch				

Thursday, July 21, 2022 – Afternoon I

13:50 – 14:00	Award Ceremony of the Journal of Complexity – Lecture Hall 1				
14:00 – 15:00	Lecture Hall 1 **Plenary Talk** ***Dmitriy Bilyk*** **On some problems of L. Fejes Tóth about point distributions on the sphere** p. 39 Chair: *Friedrich Pillichshammer*				
15:00 – 15:30	Coffee break – Halls B and C				
	Lecture Hall 1 **Technical Session** Chair: *Arne Winterhof*	Lecture Hall 3 **Technical Session** Chair: *Jan Vybíral*	Lecture Hall 4 **Technical Session** Chair: *Alexander Steinicke*	Lecture Hall 5 **Technical Session** Chair: *Stefan Thonhauser*	Lecture Hall 6 **Technical Session** Chair: *Michaela Szölgyenyi*
15:30 – 16:00	*Matthew Sutton* Concave-Convex PDMP-based samplers p. 211	*Michael Gnewuch* Hermite spaces: properties, L^2-approximation, and integration p. 121	*Szymon Urbas* Exact sequential inference for a diffusion-driven Cox process p. 218	*Sascha Desmettre* Monte Carlo simulation in the mean-field LIBOR market model p. 105	*Paul B. Rohrbach* Multilevel simulation of hard sphere mixtures p. 186
16:00 – 16:30	*Pia Stammer* Using importance sampling to speed up non-intrusive uncertainty quantification for Monte Carlo simulations p. 207	*Klaus Ritter* Equivalence of integration on Gaussian spaces and Hermite spaces p. 185	*Guo-Jhen Wu* Analysis and optimization of certain parallel Monte Carlo methods in the low temperature limit p. 232	*Lea Enzi* Numerical methods for risk functionals p. 112	*Tomohiko Hironaka* An efficient estimator of nested expectations without conditional sampling p. 130

Thursday, July 21, 2022 – Afternoon II

	Lecture Hall 1	Lecture Hall 3	Lecture Hall 4	Lecture Hall 5	Lecture Hall 6
	Special Session *Alexander D. Gilbert* and *Florian Puchhammer* Smoothing and Adaptive Methods, Part 1 of 2 p. 75 Chair: *Simon Weissman*	**Special Session** *David Krieg* and *Mario Ullrich* Approximation from Random Data, Part 2 of 2 p. 54 Chair: *Mario Ullrich*	**Special Session** *Andrea Barth* and *Andreas Stein* Multilevel and Higher-Order Approximations for Stochastic Processes, Random Fields and PDEs p. 63 Chair: *Andrea Barth*	**Special Session** *Sascha Desmettre* Simulation and Monte Carlo Methods in Quantitative Finance and Insurance p. 74 Chair: *Sascha Desmettre*	**Special Session** *Art B. Owen* and *Takashi Goda* Quasi-Monte Carlo Methods of High Order and Beyond, Part 2 of 2 p. 68 Chair: *Takashi Goda*
16:30 – 17:00	*Alexander D. Gilbert* Theory and construction of lattice rules after preintegration for pricing Asian options p. 118	*Weiwen Mo* Constructing lattice-based algorithms for multivariate function approximation with a composite number of points p. 158	*Cedric Beschle* A-posteriori numerical methods for random elliptic PDEs p. 92	*Jörn Sass* Modeling a life insurers balance sheet and analyzing its long-term stability p. 192	*Art B. Owen* Super-polynomial accuracy of median-of-means p. 166
17:00 – 17:30	*Abdul-Lateef Haji-Ali* Multilevel path branching for digital options p. 126	*Jan Vybíral* Schur's multiplication theorem and lower bounds for numerical integration p. 224	*Robin Merkle* Subordinated random fields and elliptic PDEs p. 157	*Stefan Thonhauser* Option pricing and regularity of payoffs p. 214	*Kosuke Suzuki* Component-by-component construction of randomized rank-1 lattice rules achieving almost the optimal randomized error rate p. 212

Thursday, July 21, 2022 – Afternoon III

	Lecture Hall 1	Lecture Hall 3	Lecture Hall 4	Lecture Hall 5	Lecture Hall 6
	Special Session *Alexander D. Gilbert* and *Florian Puchhammer* Smoothing and Adaptive Methods, Part 1 of 2 p. 75 Chair: *Simon Weissman*	**Special Session** *David Krieg* and *Mario Ullrich* Approximation from Random Data, Part 2 of 2 p. 54 Chair: *Mario Ullrich*	**Special Session** *Andrea Barth* and *Andreas Stein* Multilevel and Higher-Order Approximations for Stochastic Processes, Random Fields and PDEs p. 63 Chair: *Andrea Barth*	**Special Session** *Sascha Desmettre* Simulation and Monte Carlo Methods in Quantitative Finance and Insurance p. 74 Chair: *Sascha Desmettre*	**Special Session** *Art B. Owen* and *Takashi Goda* Quasi-Monte Carlo Methods of High Order and Beyond, Part 2 of 2 p. 68 Chair: *Takashi Goda*
17:30 – 18:00	*Sebastian Krumscheid* Adaptive stratified sampling for non-smooth problems p. 141	*Laurence Wilkes* A randomised lattice algorithm for integration using a fixed generating vector p. 229	*Sankarasubramanian Ragunathan* Higher-order adaptive numerical methods for computing the exit times of stochastic processes p. 177	*Jörg Wenzel* Applications of the central limit theorem for pricing cliquet-style options p. 227	*Yuya Suzuki* Scaled lattice rules for integration over $\mathbb{R}^d$ achieving higher order convergence p. 213
18:00 – 18:30	*Sifan Liu* Pre-integration via active subspaces p. 148		*Andreas Stein* MLMC-FEM for elliptic PDEs with Besov random tree coefficients p. 208	*Christian Laudagé* Severity modeling of extreme insurance claims for tariffication p. 143	
19:00 –	MCQMC Steering Committee Meeting (closed meeting) – Teichwerk				

Friday, July 22, 2022 – Morning I

	Lecture Hall 1	Lecture Hall 3	Lecture Hall 4	Lecture Hall 5	Lecture Hall 6
	Special Session *Alexander D. Gilbert* and *Florian Puchhammer* Smoothing and Adaptive Methods, Part 2 of 2 p. 75 Chair: *Alexander D. Gilbert*	**Special Session** *Gunther Leobacher* Analysis and Simulation of SDEs in Non-Standard Settings p. 52 Chair: *Gunther Leobacher*	**Special Session** *Michael Gnewuch* and *Florian Pausinger* Random Points: Generation, Quality Criteria, and Applications p. 69 Chair: *Michael Gnewuch*	**Special Session** *László Mérai* Pseudo-Random Number Generation p. 65 Chair: *László Mérai*	**Technical Session** Chair: *Kosuke Suzuki*
09:00 – 09:30	*Andrea Scaglioni* Convergence of adaptive stochastic collocation with finite elements p. 193	*Gunther Leobacher* Orthogonal projection on manifolds and numerical schemes for SDEs p. 146	*François Clément* Efficient algorithms for star discrepancy subset selection p. 101	*Vishnupriya Anupindi* Linear complexity of some sequences derived from hyperelliptic curves of genus 2 p. 85	*Jonathan Spence* Hierarchical and adaptive methods for efficient risk estimation p. 203
09:30 – 10:00	*Abirami Srikumar* Approximating distribution functions in uncertainty quantification using quasi-Monte Carlo methods p. 206	*Verena Schwarz* Regular conditional distributions for semimartingale SDEs p. 195	*Ujué Etayo* A combined use of fibrations and determinantal point processes p. 112	*Domingo Gómez-Pérez* Generating pseudorandom number sequences with Gaussian distribution p. 123	*Urbain Vaes* Mobility estimation for Langevin dynamics using control variates p. 218

Friday, July 22, 2022 – Morning II

	Lecture Hall 1	Lecture Hall 3	Lecture Hall 4	Lecture Hall 5	Lecture Hall 6
	Special Session *Alexander D. Gilbert* and *Florian Puchhammer* Smoothing and Adaptive Methods, Part 2 of 2 p. 75 Chair: *Alexander D. Gilbert*	**Special Session** *Gunther Leobacher* Analysis and Simulation of SDEs in Non-Standard Settings p. 52 Chair: *Gunther Leobacher*	**Special Session** *Michael Gnewuch* and *Florian Pausinger* Random Points: Generation, Quality Criteria, and Applications p. 69 Chair: *Michael Gnewuch*	**Special Session** *László Mérai* Pseudo-Random Number Generation p. 65 Chair: *László Mérai*	**Technical Session** Chair: *Kosuke Suzuki*
10:00 – 10:30	*Simon Weissman* A multilevel subset simulation for estimating rare events via shaking transformations p. 227	*Christoph Reisinger* Convergence of a time-stepping scheme to the free boundary in the supercooled Stefan problem p. 182	*Julian Hofstadler* Consistency of randomized integration points p. 131	*Pierre Popoli* Maximum order complexity for some automatic and morphic sequences along polynomial values p. 173	*Alessandro Mastrototaro* AdaSmooth: a fast and stable SMC algorithm for online additive smoothing p. 156
10:30 – 11:00		*Alexander Steinicke* From numerical schemes for SDEs to analysis of Lipschitz maps p. 210	*Markus Kiderlen* Stratified and jittered sampling in discrepancy theory p. 138	*Arne Winterhof* Pseudorandom sequences derived from automatic sequences p. 230	
11:00 – 11:30	Coffee break – Halls B and C				
11:30 – 12:30	Lecture Hall 1 **Plenary Talk** ***Ian H. Sloan*** **Periodicity oils the wheels—periodicity, QMC and uncertainty quantification** p. 45 Chair: *Peter Kritzer*				
12:30 – 12:35	Closing Remarks – Lecture Hall 1				

Sunday Tutorials

Sunday, July 17, 2022, 14:15 – 15:45, Lecture Hall 1

Further applications of quasi-Monte Carlo Methods to PDEs with random coefficients

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In recent years the modern quasi-Monte Carlo (QMC) theory has been successfully applied to a number of applications involving PDEs with random coefficients. This tutorial will showcase some ongoing works which continue to take QMC methods to new territories, including: a revolutionary approach to modelling random fields using periodic random variables; a fast kernel-based lattice-point interpolation; a parabolic PDE-constrained optimal control problem under uncertainty with entropic risk measure; an approximation of distribution functions and densities with smoothing by preintegration; and a Poisson equation on random domains via the domain mapping approach.

The common and essential theme among these collaborations with various international teams is that we are not just applying an off-the-shelf QMC method; rather, we provide rigorous error and cost analysis to design QMC methods tailored to the features of the underlying mathematical functions in these applications. This tutorial will explain some of the proof techniques used for various components of the analysis.

Sunday, July 17, 2022, 16:00 – 17:30, Lecture Hall 1

Sampling with Stein Discrepancies

Chris J. Oates
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As a statistical paradigm, Bayesian inference is conceptually simple and elegant. However, the computational challenge of sampling from the posterior distribution represents a major practical restriction on the class of models that can be analysed. Stein's method has recently emerged as a powerful tool in computational statistics, being used to construct novel sampling methods that have, in certain situations, out-performed the state-of-the-art. This tutorial will explain how Stein's method can be used to transform a sampling problem into an optimisation problem, before introducing several different optimisation algorithms that each give rise to a practical computational method for Bayesian inference.

The main technical tool that we use is *Stein discrepancy*, and some of the interesting open theoretical and methodological challenges associated with Stein discrepancy will be highlighted.

Plenary Talks

Wednesday, July 20, 2022, 09:00 – 10:00, Lecture Hall 1

Uncertainty quantification with discontinuous random fields

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Coauthor(s): Andreas Stein, Robin Merkle, Cedric Beschle

General elliptic equations with spatially discontinuous diffusion coefficients may be used as a simplified model for subsurface flows in heterogeneous or fractured porous media. In the model, data sparsity and measurement errors are often taken into account by a randomization of the diffusion coefficient of the elliptic equation highlighting the necessity of the construction of flexible, spatially discontinuous random fields. Lévy fields and subordinated random fields are random functions on higher dimensional parameter domains with discontinuous sample paths and great distributional flexibility. In this talk, we introduce various ways to construct discontinuous random fields and consider a random elliptic partial differential equation where the discontinuous random fields occur in the diffusion coefficient. Problem specific multilevel Monte Carlo Finite Element methods are constructed to approximate the mean of the solution to the random elliptic PDE accounting for the reduced stochastic and spacial regularity of the coefficient and, hence, the solution to the PDE.

Thursday, July 21, 2022, 14:00 – 15:00, Lecture Hall 1

On some problems of L. Fejes Tóth about point distributions on the sphere

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In addition to proving a myriad of important results, László Fejes Tóth has posed a number of interesting questions and conjectures about point distributions on the sphere, many of which are open to this day and some have been solved recently. These problems include, in particular, finding point distributions which maximize various discrete energies (sum of Euclidean distances, sum of geodesic distances, sum of acute angles etc), covering the sphere by spherical zones of optimal width, non-uniformity of tessellations of the sphere by hyperplanes etc. In the talk, we shall explore these questions as well as their history and the exciting mathematics that arises in connection to them: Stolarsky principle relating discrepancy and sum of distances, positive definite functions and the linear programing method for energy optimization, the Sylvester-Gallai theorem, energies with discrete minimizers, one-bit sensing etc.

Wednesday, July 20, 2022, 15:30 – 16:30, Lecture Hall 1

A quasi-Monte Carlo data compression algorithm for machine learning

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Coauthor(s): Josef Dick

We present an algorithm from [1] to reduce large data sets using so-called digital nets, which are well distributed point sets in the unit cube. The algorithm efficiently scans the data and computes certain data dependent weights. Those weights are used to approximately represent the data, without making any assumptions on the distribution of the data points. Under smoothness assumptions on the model, we then show that this can be used to reduce the computational effort needed in finding good parameters in machine learning problems which aim to minimize quantities of the form

$$\min_{\theta} \frac{1}{n} \sum_{i=1}^{n} (f_\theta(x_i) - y_i)^2.$$

While the principal idea of the approximation might also work with other point sets, the particular structural properties of digital nets can be exploited to make the computation of the necessary weights extremely fast.

[1] J. Dick, M. Feischl, A quasi-Monte Carlo data compression algorithm for machine learning, Journal of Complexity, Volume 67, 2021.

Tuesday, July 19, 2022, 14:00 – 15:00, Lecture Hall 1

MLMC techniques for discontinuous functions

Mike Giles
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Multilevel Monte Carlo (MLMC) techniques for estimating scalar quantities of the form $\mathbb{E}[f(U)]$ rely on an intermediate quantity U being approximated with increasing accuracy, and increasing cost, on a sequence of levels. If the function f is Lipschitz, this leads to increasingly small differences in the approximations to $f(U)$, and the resulting low variance for these differences is central to the effectiveness of MLMC, with very few samples needed on the finest levels of correction [2].

In this talk I will discuss the challenges which arise when the function f is discontinuous, which can lead to a much slower decay in the variance of the MLMC correction. I will review the existing literature on techniques which can be used to overcome these challenges in a variety of different contexts, and discuss recent developments using either a branching diffusion or adaptive sampling:

- smoothing [2,5]
- integration [1,7]
- conditional expectation [2]
- change of measure [2,8]
- splitting [2,3]
- adaptive sampling [4,6]

[1] M. Altmayer, A. Neuenkirch. 'Multilevel Monte Carlo quadrature of discontinuous payoffs in the generalized Heston model using Malliavin integration by parts'. *SIAM Journal on Financial Mathematics*, 6(1):22-52, 2015.

[2] M.B. Giles. 'Multilevel Monte Carlo methods'. *Acta Numerica*, 24:259-328, 2015.

[3] M.B. Giles, F. Bernal. 'Multilevel estimation of expected exit times and other functionals of stopped diffusions'. *SIAM/ASA Journal on Uncertainty Quantification*, 6(4):1454-1474, 2018.

[4] M.B. Giles, A.-L. Haji-Ali. 'Multilevel nested simulation for efficient risk estimation'. *SIAM/ASA Journal on Uncertainty Quantification*, 7(2):497-525, 2019.

[5] M. Giles, T. Nagapetyan, K. Ritter. 'Multilevel Monte Carlo approximation of distribution functions and densities'. *SIAM/ASA Journal on Uncertainty Quantification*, 3:267-295, 2015.

[6] A.-L. Haji-Ali, J. Spence, A. Teckentrup. 'Adaptive multilevel Monte Carlo for probabilities'. arXiv:2107.09148.

[7] S. Krumscheid, F. Nobile. 'Multilevel Monte Carlo approximation of functions'. *SIAM/ASA Journal on Uncertainty Quantification*, 6(3):1256-1293, 2018.

[8] Y. Xia, M.B. Giles. 'Multilevel path simulation for jump-diffusion SDEs', pp.695-708 in *Monte Carlo and Quasi-Monte Carlo Methods 2010*, Springer, 2012.

Monday, July 18, 2022, 14:00 – 15:00, Lecture Hall 1

Sampling via stochastic localization

Andrea Montanari
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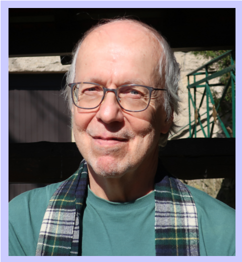
Coauthor(s): Ahmed El Alaoui, Mark Sellke, Yuchen Wu

Stochastic localization refers to a class of a martingale processes indexed by time and taking values in the space of probability measures over $\mathbb{R}^n$. This notion was introduced by Ronen Eldan as a technique to prove functional inequalities for certain classes of probability measures. I will provide a simple self-contained introduction to this construction, and then show how it can be implemented algorithmically, at least in certain cases. When this is possible, stochastic localization offers an interesting alternative to MCMC methods. I will discuss two examples in which this yields provably efficient sampling algorithms for problems in which this was not known before.

Thursday, July 21, 2022, 09:00 – 10:00, Lecture Hall 1



Optimal algorithms for numerical integration: recent results and open problems

Erich Novak
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We present recent results on optimal algorithms for numerical integration and several open problems. The talk has, after an introduction, four parts:

1. Two Lower Bounds,
2. Universality,
3. General Domains,
4. iid Information.

For references see the arXiv. Recent coauthors: Aicke Hinrichs, David Krieg, Robert Kunsch, Joscha Prochno, Daniel Rudolf, Mathias Sonnleitner, Mario Ullrich, Jan Vybíral, Henryk Woźniakowski and Shun Zhang.

Friday, July 22, 2022, 11:30 – 12:30, Lecture Hall 1

Periodicity oils the wheels—periodicity, QMC and uncertainty quantification

Ian H. Sloan
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Since the invention of Quasi-Monte Carlo integration mid-twentieth century, there have always been two versions of QMC: the periodic, associated with Korobov, Bahvalov, Zaremba, Hua and others; and the non-periodic, associated with Halton, Hlawka, Sobol, and more recently Niederreiter, Dick and others. The periodic setting offers the profound benefits of Fourier series, but has been lacking in serious high-dimensional applications. After a review of integration in the periodic setting, I will describe the recent development of a periodic QMC method for high-dimensional approximation (as distinct from integration) in the context of uncertainty quantification. In this problem an elliptic partial differential equation with a random input field is modelled in a non-standard way with periodic random variables. The claim to high-dimensional applicability is based on a computational cost that grows merely linearly with dimensionality. Collaborators in this work are Vesa Kaarnioja, Yoshihito Kazashi, Frances Kuo and Fabio Nobile. The work rests, of course, on the contributions of numerous others, including Cools, Hickernell, Nuyens, Woźniakowski, . . .

Tuesday, July 19, 2022, 09:00 – 10:00, Lecture Hall 1

Error estimates and variance reduction for nonequilibrium stochastic dynamics

Gabriel Stoltz
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Equilibrium properties in statistical physics are obtained by computing averages with respect to Boltzmann–Gibbs measures, sampled in practice using ergodic dynamics such as the Langevin dynamics. Some quantities however cannot be computed by simply sampling the Boltzmann–Gibbs measure, in particular transport coefficients, which relate the current of some physical quantity of interest with the forcing needed to induce it. For instance, a temperature difference induces an energy current, the proportionality factor between these two quantities being the thermal conductivity. From an abstract point of view, transport coefficients can also be considered as some form of sensitivity analysis with respect to an added forcing to the baseline dynamics.

There are various numerical techniques to estimate transport coefficients, which all suffer from large errors, in particular large statistical errors. I will review the most popular methods, namely the Green–Kubo approach where the transport coefficient is rewrittten as some time-integrated correlation function, and the approach based on longtime averages of the stochastic dynamics perturbed by an external driving (so-called nonequilibrium molecular dynamics). I will make precise in each case the various sources of errors, in particular the bias related to the time discretization of the underlying continuous dynamics, and the variance of the associated Monte Carlo estimators. I will also briefly present some recent alternative techniques to estimate transport coefficients.

Monday, July 18, 2022, 09:00 – 10:00, Lecture Hall 1

Gaussian process regression in inverse problems and Markov chain Monte Carlo

Aretha Teckentrup
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Coauthor(s): Tianming Bai, Konstantinos Zygalakis

We are interested in the inverse problem of estimating unknown parameters in a mathematical model from observed data. We follow the Bayesian approach, in which the solution to the inverse problem is the distribution of the unknown parameters conditioned on the observed data, the so-called posterior distribution. We are particularly interested in the case where the mathematical model is non-linear and expensive to simulate, for example given by a partial differential equation.

A major challenge in the application of sampling methods such as Markov chain Monte Carlo is then the large computational cost associated with simulating the model for a given parameter value. To overcome this issue, we consider using Gaussian process regression to approximate the likelihood of the data. This results in an approximate posterior distribution, to which sampling methods can be applied with feasible computational cost.

In this talk, we will show how the uncertainty estimate provided by Gaussian process regression can be incorporated into the approximate Bayesian posterior distribution to avoid overconfident predictions, and present efficient Markov chain Monte Carlo methods in this context.

Special Sessions

Advanced Particle Methods for Bayesian Inference

Organizers:

Neil K. Chada
King Abdullah University of Science and Technology
neilchada123@gmail.com

Simon Weissmann
University of Heidelberg
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Session Description:

The understanding and incorporation of data within models has become a vital component of applied mathematics. A fundamental task one can ask is given noisy measurements of data, how to recover some unknown quantity of interest. Some examples of these fields include inverse problems which is primarily concerned with parameter estimation and data assimilation for state estimation. Both fields have seen a considerable amount of attention due to recent advancements in terms of both classical and statistical approaches. In particular, this mini-symposium will consider particle methods for solving inverse problems with the help optimization tools as well as particle methods aiming to represent the posterior distribution in a bayesian point of view for inverse problems.

The motivation behind this mini-symposium is to bring together experts from both schools. This would provide a complimentary field to the mini-symposium where connections between both areas are currently being developed.

Thursday, July 21, 2022, 10:30 – 12:30, Lecture Hall 4

Gottfried Hastermann
Analysis of a localized non-linear ensemble Kalman–Bucy filter with sparse observations p. 128

Sahani Pathiraja
Theoretical insights on a class of control based particle filters and their approximations p. 169

Tim Roith
A kernelized consensus-based optimization method p. 187

Björn Sprungk
Dimension-independent Markov chain Monte Carlo on the sphere p. 205

Algorithmic Advancements in MCQMC Software

Organizer:

Pieterjan Robbe
Sandia National Laboratories
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Session Description:

Converting novel (Q)MC algorithms into efficient and easy-to-use software is crucial to ensure further community engagement. The talks in this special session will present several recently developed algorithms from the MCQMC community, including examples of *best practices* on how these algorithms can either be integrated into existing software packages, or turned into new software.

Tuesday, July 19, 2022, 10:30 – 12:30, Lecture Hall 5

Dirk Nuyens
An adaptive algorithm for integration on $\mathbb{R}^d$ using lattice rules p. 164

Aleksei Sorokin
Quasi-Monte Carlo for vector functions of integrals p. 200

Linus Seelinger
Connecting advanced models and advanced UQ: the MIT UQ library (MUQ) and a universal UQ/model interface p. 196

Alexander Keller
Quasi-Monte Carlo algorithms (not only) for graphics software p. 137

Analysis and Simulation of SDEs in Non-Standard Settings

Organizer:

Gunther Leobacher
University of Graz
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Session Description:

In recent years applications have increasingly been demanding stochastic models that transcend classical results on existence, uniqueness and numerical approximation of stochastic differential equations (SDEs). In this session we present recent results related to SDEs in non standard settings, like non-Lipschitz drift, degenerate diffusion, or non-standard driving processes.

Friday, July 22, 2022, 09:00 – 11:00, Lecture Hall 3

Approximate Models for Rare Event Simulation and Uncertainty Quantification

Organizer:

Frédéric Cérou
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Session Description:

Particle or population based algorithms to simulate rare events are now well established. If we consider an event of the form $P(\phi(X) > L)$, with some random vector X, real function ϕ and real L, these algorithms need a lot of calls to the function ϕ. In many real life applications however, the function ϕ is very costly to evaluate (e.g. the solution of a PDE taking X as parameters), and we would like to replace it, as often as possible, by some approximate or surrogate function much easier to compute. How to do that efficiently, and what gain to expect in doing so, are the core topic of this session.

The first talk will be given by Arnaud Guyader (Sorbonne University, Paris), giving an optimal and recursive approach when ϕ is Lipschitz.

Frédéric Cérou (Inria & Univ Rennes) will consider a case with surrogate models available, with an approach based on Kullback-Leibler divergence to recursively select reduced order models and nested events.

Maliki Moustapha (ETH, Zürich) will present how active learning can constrain the surrogate limit-state function to be accurate only in some regions of interest and hence reduce the computational cost. He will also present related numerical results on an extensive benchmark.

Elisabeth Ullmann (TUM, München) will consider the PDE case, and address two main points: (1) the impact of the PDE approximation error on the failure probability estimate, and (2) the use of the Ensemble Kalman Filter for the estimation of failure probabilities.

Wednesday, July 20, 2022, 10:30 – 12:30, Lecture Hall 5

Approximation from Random Data

Organizers:

David Krieg
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Mario Ullrich
JKU Linz
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Session Description:

This session is concerned with approximation problems like function recovery, compressed sensing, and the computation of norms and integrals. In many situations, an active acquisition of data is impossible and only random data is available. For this reason, we would like to bring together experts who contributed to the theory of algorithms based on random data from different perspectives. This includes error analysis for high-dimensional problems, discretization in function spaces and modern methods in data science.

Part 1	Thursday, July 21, 2022, 10:30 – 12:30, Lecture Hall 3

Part 2	Thursday, July 21, 2022, 16:30 – 18:30, Lecture Hall 3

Developments in and Applications of MCQMC Software

Organizer:

Fred J. Hickernell
Illinois Institute of Technology
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Session Description:

There are several initiatives to turn the best MCQMC algorithms into efficient, robust, user-friendly software. This is done to 1) promote the application of MCQMC, 2) provide a platform for theoreticians to showcase their algorithms, and 3) facilitate the comparison of different algorithms. This special session highlights the latest developments in some new and existing MCQMC software packages.

Part 1	Monday, July 18, 2022, 10:30 – 12:30, Lecture Hall 5

Mike Giles
Progress on MATLAB and C/C++ implementations of an MLMC package p. 119

Pierre L'Ecuyer
An update on Lattice Tester, LatMRG, and Lattice Builder p. 145

Fred J. Hickernell
Challenges in developing great MCQMC software p. 130

Loïs Paulin
Generator matrices by solving integer linear programs p. 170

Part 2	Monday, July 18, 2022, 16:30 – 18:00, Lecture Hall 5

Emil Løvbak
Reversible random number generators and adjoint Monte Carlo simulation for tokamak divertor design p. 150

Pieterjan Robbe
Bayesian calibration for summary statistics with applications to a cluster dynamics model p. 185

Vince Maes
Hybrid deterministic/MC methods in SOLPS-ITER p. 154

Developments in Markov Chain Monte Carlo

Organizer:

Vivekananda Roy
Iowa State University
vroy@iastate.edu

Session Description:

Markov chain Monte Carlo (MCMC) methods are being actively explored for effective use of Bayesian methodology in increasingly complex and large data problems. The four presentations in this proposed session look at finding efficient computational methods and their properties including convergence diagnostics and variance estimation as well as reduction. Thus the session covers recent research developments in MCMC computing including advances in theory, as well as methodology. There is no discussant because we first want to get the material out into the general community.

Monday, July 18, 2022, 10:30 – 12:30, Lecture Hall 4

Alain Durmus
The Kick-Kac teleportation algorithm: boost your favorite Markov Chain Monte Carlo using Kac formula p. 110

James M. Flegal
Lugsail lag windows for estimating time-average covariance matrices p. 117

Leah F. South
Monte Carlo variance reduction using Stein operators p. 201

Andrej Srakar
Approximate Bayesian algorithm for tensor robust principal component analysis p. 205

Energy-minimizing Point Configurations and Measures I

Organizers:

Dmitriy Bilyk
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Ryan W. Matzke
Graz University of Technology
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Session Description:

The last few years have seen an increased interest in optimizing the variational functionals of the form

$$I_F(\mu) := \iint_\Omega F(x,y)\, d\mu(x) d\mu(y), \qquad \operatorname{supp}\mu \subset \Omega \subset \mathbb{R}^{\mathrm{d}},$$

acting on probability measures supported in a compact set Ω. The properties of I_F that were investigated include the characterization of the ground state measures, their applications to point distribution, and dynamics of the gradient flows of I_F, among others. This interest is motivated partly by the connections to discrepancy theory, geometry of line and point packings on the sphere, and partly by the applications in flocking, emergent behavior, and mathematical physics. In this special session we propose to bring together researchers from different groups, working on various aspects of the functionals I_F, in order to facilitate collaboration and scientific contacts.

[1] Bäuml, L., Finster, F., Schiefeneder, D., & von der Mosel, H. (2019). *Singular support of minimizers of the causal variational principle on the sphere.* Calculus of Variations and Partial Differential Equations, 58(6), 127.

[2] Beltrán, C., Marzo, J., & Ortega-Cerdà, J. (2016). Energy and discrepancy of rotationally invariant determinantal point processes in high dimensional spheres. Journal of Complexity, 37, 76109. doi:10.1016/j.jco.2016.08.001

[3] Bilyk, D., & Dai, F. (2019). Geodesic distance Riesz energy on the sphere. Transactions of the American Mathematical Society, 372(5), 31413166.

[4] Bilyk, D., Dai, F., & Matzke, R. (2018). The Stolarsky Principle and Energy Optimization on the Sphere. Constructive Approximation, 48(1), 3160. doi:10.1007/s00365-017-9412-4

[5] Bilyk, D., Matzke, R., & Vlasiuk, O. (2021). Positive definiteness and the Stolarsky invariance principle. arXiv: 2110.04138.

[6] Carrillo, J. A., Figalli, A., & Patacchini, F. S. (2017). Geometry of minimizers for the interaction energy with mildly repulsive potentials. Annales de lInstitut Henri Poincare (C) Non Linear Analysis, 34(5), 12991308. doi:10.1016/j.anihpc.2016.10.004

[7] Finster, F., & Schiefeneder, D. (2013). *On the Support of Minimizers of Causal Variational Principles.* Archive for Rational Mechanics and Analysis, 210(2), 321364. doi:10.1007/s00205-013-0649-1

[8] Marzo, J., & Mas, A. (2019). Discrepancy of minimal Riesz energy points. arXiv: 1907.04814.

[9] Skriganov, M. M. (2019). Point distributions in two-point homogeneous spaces. Mathematika, 65(3), 557587.

Tuesday, July 19, 2022, 10:30 – 12:00, Lecture Hall 3

Energy-minimizing Point Configurations and Measures II

Organizers:

Tetiana Stepaniuk
University of Lübeck
`stepaniuk@math.uni-luebeck.de`

Oleksandr Vlasiuk
Vanderbilt University
`oleksandr.vlasiuk@vanderbilt.edu`

Session Description:

The last few years have seen an increased interest in optimizing the variational functionals of the form

$$I_F(\mu) := \iint_\Omega F(x,y)\, d\mu(x) d\mu(y), \qquad \operatorname{supp}\mu \subset \Omega \subset \mathbb{R}^{\mathrm{d}},$$

acting on probability measures supported in a compact set Ω. The properties of I_F that were investigated include the characterization of the ground state measures, their applications to point distribution, and dynamics of the gradient flows of I_F, among others. This interest is motivated partly by the connections to discrepancy theory, geometry of line and point packings on the sphere, and partly by the applications in flocking, emergent behavior, and mathematical physics. In this special session we propose to bring together researchers from different groups in Europe and the US, working on various aspects of the functionals I_F, in order to facilitate collaboration and scientific contacts.

This session is intended as part of a double session, with the first part being "Energy-minimizing Point Configurations and Measures I" organized by Dmitriy Bilyk and Ryan W. Matzke.

[1] Bäuml, L., Finster, F., Schiefeneder, D., & von der Mosel, H. (2019). *Singular support of minimizers of the causal variational principle on the sphere.* Calculus of Variations and Partial Differential Equations, 58(6), 127.

[2] Beltrán, C., Marzo, J., & Ortega-Cerd, J. (2016). Energy and discrepancy of rotationally invariant determinantal point processes in high dimensional spheres. Journal of Complexity, 37, 76109. doi:10.1016/j.jco.2016.08.001

[3] Bilyk, D., & Dai, F. (2019). Geodesic distance Riesz energy on the sphere. Transactions of the American Mathematical Society, 372(5), 31413166.

[4] Bilyk, D., Dai, F., & Matzke, R. (2018). The Stolarsky Principle and Energy Optimization on the Sphere. Constructive Approximation, 48(1), 3160. doi:10.1007/s00365-017-9412-4

[5] Bilyk, D., Matzke, R., & Vlasiuk, O. (2021). Positive definiteness and the Stolarsky invariance principle. arXiv: 2110.04138.

[6] Carrillo, J. A., Figalli, A., & Patacchini, F. S. (2017). Geometry of minimizers for the interaction energy with mildly repulsive potentials. Annales de lInstitut Henri Poincare (C) Non Linear Analysis, 34(5), 12991308. doi:10.1016/j.anihpc.2016.10.004

[7] Finster, F., & Schiefeneder, D. (2013). *On the Support of Minimizers of Causal Variational Principles*. Archive for Rational Mechanics and Analysis, 210(2), 321364. doi:10.1007/s00205-013-0649-1

[8] Marzo, J., & Mas, A. (2019). Discrepancy of minimal Riesz energy points. arXiv: 1907.04814.

[9] Skriganov, M. M. (2019). Point distributions in two-point homogeneous spaces. Mathematika, 65(3), 557587.

Tuesday, July 19, 2022, 16:30 – 18:00, Lecture Hall 3

Laplace Approximation and Other Model-Based Preconditioning Methods for Monte Carlo Algorithms

Organizers:

Claudia Schillings
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Philipp Wacker
FAU Erlangen-Nürnberg
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Session Description:

Various numerical procedures, and in particular Monte Carlo methods like Importance Sampling and Markov chain Monte Carlo in high-dimensional problems, suffer from the fact that the parameter set most relevant for the computation is concentrated on a small subset. A prime example is the Bayesian inference setting with highly informative data, which leads to a strong concentration of the posterior with respect to the prior, and performance issues for sampling algorithms. This problem can be alleviated by the employment of preconditioners, for example based on variational approaches or the Laplace approximation, and adaptive exploration of the parameter space. In this session we will discuss various aspects of this topic, starting with well-definedness of the concept of MAP estimators (which is highly relevant for preconditioners centered around a mode of the posterior distribution), to approximation properties of the Laplace method, and computational performance of Monte Carlo algorithms focussing on a parameter subset with high probability of the target measure.

Tuesday, July 19, 2022, 16:30 – 18:30, Lecture Hall 6

Monte Carlo Methods and Variance Reduction Techniques for Forward and Inverse Problems for Stochastic Reaction Networks

Organizers:

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Raúl Tempone
RWTH Aachen University, King Abdullah University of Science and Technology
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Session Description:

Stochastic reaction networks (SRNs) are a class of continuous-time Markov chains used to model many real-life phenomena, such as the time-evolution of biological and chemical reactions, epidemics, risk theory, and queuing networks. In this mini-symposium, we are interested in the recent advances related to Monte Carlo methods and variance reduction techniques for solving forward and inverse problems in the context of SRNs, in particular the efficient estimation of related statistical quantities. We present the recent improvements of Monte Carlo, multilevel Monte Carlo, and quasi-Monte Carlo methods in this context.

Thursday, July 21, 2022, 10:30 – 12:00, Lecture Hall 5

Muruhan Rathinam
State and parameter estimation from partial state observations in stochastic reaction networks p. 178

Zhou Fang
Stochastic filtering for multiscale stochastic reaction networks based on hybrid approximations p. 113

Sophia Wiechert
Efficient importance sampling via stochastic optimal control for stochastic reaction networks p. 228

Multilevel and Higher-Order Approximations for Stochastic Processes, Random Fields and PDEs

Organizers:

Andrea Barth
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Andreas Stein
ETH Zürich
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Session Description:

Uncertainty quantification plays an increasingly important role in a wide range of problems in the natural sciences and financial mathematics. The underlying model may be subject to various uncertainties such as parameter or domain uncertainty, model uncertainty, numerical errors, or some intrinsic stochastic variability of the model. Advanced numerical methods such as adaptive or higher-order methods are needed to lower computational complexity or even be able to numerically solve complex stochastic models.

This special session aims at bringing together advanced numerical methods to solve problems in stochastic analysis and uncertainty quantification.

Thursday, July 21, 2022, 16:30 – 18:30, Lecture Hall 4

Periodic Point Configurations and Lattice Point Interactions

Organizers:

Johann S. Brauchart
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Peter J. Grabner
Graz University of Technology
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Session Description:

The *packing density* of an infinite point configuration X (assuming that $\forall x, y \in X : x \neq y \Rightarrow \|x - y\| \geq 1$) inEuclidean space is given by

$$\liminf_{R\to\infty} \frac{\lambda_d\left(\bigcup_{x\in X\cap B(0,R)} B(x,1)\right)}{\lambda_d(B(0,R))}.$$

Cohn, Kumar, Miller, Radchenko, and Viazovska recently have made a major progress in the determination of the best packing configurations in dimensions 8 and 24. Very recently, a further important step has been made by the same group of authors in proving the universal optimality of the E_8 and the Leech lattice in these dimensions. Universal optimality refers to the fact that these lattices minimise the p-energy

$$\sum_{\substack{\mathbf{x}\in\Lambda\\ \mathbf{x}\neq\mathbf{0}}} p(\|\mathbf{x}\|)$$

for all completely monotonic functions $p : \mathbb{R}^+ \to \mathbb{R}$.

Monday, July 18, 2022, 16:30 – 18:00, Lecture Hall 3

Johann S. Brauchart
Lattice points to the sphere: towards discrepancy estimates p. 95

Laurent Bétermin
Minimality results for the Embedded-atom model p. 92

Markus Faulhuber
Optimal sampling strategies in time-frequency analysis p. 114

Pseudo-Random Number Generation

Organizer:

László Mérai
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Session Description:

Pseudo-random sequences, that is, sequences which are generated by deterministic algorithms but possess randomness properties are crucial in the application of any quasi-Monte Carlo method. The investigation of pseudo-random number generators requires both detailed studies of different measures or tests of randomness and deep analysis of individual number generators in terms of such measures. The goal of this session is to present the recent trends in pseudo-random generation in particular with a focus on applications of quasi-Monte Carlo methods.

Friday, July 22, 2022, 09:00 – 11:00, Lecture Hall 5

Quantifying Notions of Equidistribution on the Sphere

Organizers:

Damir Ferizović
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Michelle Mastrianni
University of Minnesota
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Session Description:

The problem of distributing points on the sphere $\mathbb{S}^d$ arises in a number of settings in numerical analysis and approximation theory. An integral of a function f on $\mathbb{S}^d$ is typically approximated by weighted sums of f: if $\{\mathbf{x}_j\}_{j=1}^N$ is a (nice enough) set of N points on $\mathbb{S}^d$,

$$\int_{\mathbb{S}^d} f(\mathbf{x}) d\sigma(\mathbf{x}) \approx \frac{1}{N} \sum_{j=1}^{N} f(\mathbf{x}_j).$$

Such a point set has good distribution if the error for numerical integration is small for some class of functions. The numerical integration error for random point sets will be the subject of a talk in this session by J. Marzo.

One approach to studying the distribution of a point set is via the spherical cap discrepancy. In [1] it is shown that for i.i.d. random point sets, spherical digital nets, and spherical Fibonacci lattices, the spherical cap discrepancy is at most of order $N^{-1/2}$. Further such examples include the HEALPix lattice points, which were shown in [2] to have spherical cap discrepancy of order $N^{-1/2}$. M. Mastrianni plans to speak on this work.

Another approach to achieving good point sets on the sphere is to optimize an energy. The logarithmic energy will be the topic of talks by F. Lizarte and S. Steinerberger. Minimizers of this potential are called elliptic Fekete points and are related to Smale's 7th problem [3].

Our session aims to bring together young and senior researchers working in these subtopics of point distributions. Two PhD students and two professors will give talks in the session.

References.

[1] C. Aistleitner, J.S. Brauchart and J. Dick. *Point Sets on the Sphere* $\mathbb{S}^2$ *with Small Spherical Cap Discrepancy.* Discrete Comput Geom 48 (2012).

[2] D. Ferizović, J. Hofstadler and M. Mastrianni. *The spherical cap discrepancy of HEALPix points*, Preprint (2022).

[3] S. Smale, *Mathematical problems for the next century*, Mathematics: Frontiers and perspectives, Amer. Math. Soc., Providence, RI, pp. 271294 (2000).

Monday, July 18, 2022, 10:30 – 12:00, Lecture Hall 3

Quasi-Monte Carlo Methods of High Order and Beyond

Organizers:

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Takashi Goda
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Session Description:

This special session is devoted to quasi-Monte Carlo (QMC) methods which achieve faster decay rate of the deterministic error than $O(1/N)$ in various problem settings including high-dimensional numerical integration, approximation, and density estimation. We also consider randomized QMC methods, for which the root mean squared error can decay faster than $O(1/N)$ under an appropriate randomization of well-structured QMC point sets. The key ingredients of such *higher order QMC methods* lie in how to exploit the properties of functions (such as periodicity and smoothness) adequately and also in how to construct and randomize the underlying QMC point sets. Recently many interesting and different approaches have been developed and applied. In this special session, we bring together expertise in this active area to discuss the newest research results on QMC methods of higher order and beyond.

Part 1	Thursday, July 21, 2022, 10:30 – 12:30, Lecture Hall 6

Part 2	Thursday, July 21, 2022, 16:30 – 18:00, Lecture Hall 6

Random Points: Generation, Quality Criteria, and Applications

Organizers:

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Florian Pausinger
Queen's University Belfast
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Session Description:

Random point sets and random processes play an important role in stochastic simulation, numerical integration, optimization 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., small variance (in stochastic simulation) or low discrepancy (in quasi-Monte Carlo (QMC) integration). In this special session we want to bring together researchers from applied probability theory and from discrepancy theory to discuss different quality criteria for random point sets, the generation of good point sets, and their numerical performance in applications.

Friday, July 22, 2022, 09:00 – 11:00, Lecture Hall 4

Recent Advances in MCMC Sampling Techniques

Organizers:

Juan Pablo Madrigal Cianci
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Björn Sprungk
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Session Description:

Markov chain Monte Carlo (MCMC) methods have long been established as the gold standard in computational statistics. Due to modern computational facilities and advances in computational techniques, MCMC sampling has become feasible for more challenging inference problems arising in science and engineering. However, the development and analysis of efficient and robust algorithms for MCMC is still a very active field. Contemporary topics are, for instance, multilevel MCMC methods exploiting a hierarchy of coarse and fine approximations to the posterior, suitable MCMC methods for sampling on Riemannian manifolds, pseudo-marginal MCMC for intractable likelihoods, and advances in the convergence analysis of Markov chains. In this mini-symposium, we bring together experts working on the aforementioned problems to discuss recent advances in this field.

Tuesday, July 19, 2022, 16:30 – 18:30, Lecture Hall 4

Mareike Hasenpflug
Geodesic slice sampling on the sphere p. 128

Mikkel Bue Lykkegaard
Multilevel delayed acceptance: ergodic MCMC for model hierarchies p. 152

Katharina Schuh
Convergence of unadjusted Hamiltonian Monte Carlo for mean-field models p. 195

Andi Q. Wang
Comparison of Markov chains via weak Poincaré inequalities with application to pseudo-marginal MCMC p. 225

Recent Advances in Piecewise Deterministic Monte Carlo Methods

Organizer:

Andrea Bertazzi
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Session Description:

Piecewise deterministic Markov processes (PDMPs) have emerged as a new way to construct MCMC algorithms. Importantly, PDMPs can be designed to include a natural notion of momentum, which can improve the performance of these algorithms drastically. The theory behind such processes has seen tremendous advances in recent years. On the other hand, research on the applicability of PDMPs to real world problems has lagged behind the numerous theoretical developments. Some of the important questions in this direction are addressed in this session. In particular, the focus is on themes such as finding efficient ways to implement these algorithms, understanding their robustness, and the application to problems that arise in Bayesian statistics, as for example piecewise continuous target distributions and infinite dimensional problems.

Tuesday, July 19, 2022, 10:30 – 12:30, Lecture Hall 6

Paul Dobson
Infinite dimensional piecewise deterministic Markov processes p. 108

Sebastiano Grazzi
PDMP samplers for constrained spaces and discontinuous targets p. 123

Giorgos Vasdekis
Zig-Zag for approximate Bayesian computation p. 222

Andrea Bertazzi
Higher order approximations of piecewise deterministic Markov processes with splitting schemes p. 91

Recent Advances in Unbiased Estimation Techniques

Organizer:

Celia García-Pareja
École Polytechnique Fédérale de Lausanne
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Session Description:

Monte Carlo methods are the gold standard when it comes to estimation of expectations, and analytical expressions of the model under study are too difficult to approach or simply unavailable. A main advantage of Monte Carlo simulation is that it yields unbiased estimators, provided an exact sampling method for the underlying stochastic model exists. Such exact methods, however, are often unavailable, and the bias stemming from approximation errors is difficult to estimate. It is in these contexts that unbiased estimation techniques have attracted a lot of attention. Some examples include exact simulation of time-continuous stochastic processes of diffusion type, perfect sampling from steady-state distributions of stochastic processes, unbiased estimators for differential equations that can only be solved approximately, or, in Bayesian settings, unbiased estimators of expectations w.r.t. invariant measures of Markovian processes. This special session will offer the opportunity to walk through recent advances in the field.

Wednesday, July 20, 2022, 10:30 – 12:30, Lecture Hall 4

Ajay Jasra
On unbiased score estimation for partially observed diffusions p. 134

Karthyek Murthy
Exact simulation of multidimensional reflected Brownian motion p. 162

Willem van den Boom
Unbiased approximation of posteriors via coupled particle Markov chain Monte Carlo p. 219

Shangda Yang
Multi-index sequential Monte Carlo and randomized multi-index sequential Monte Carlo ratio estimators p. 234

Robust Innovations in Gradient-Based MCMC

Organizer:

Chris Sherlock
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Session Description:

Metropolis-Hastings algorithms with proposals informed by the local gradient have long been known to perform substantially better in high dimensions than simpler alternatives such as the random-walk Metropolis and independence sampler. In particular, Hamiltonian Monte Carlo (HMC) and the Metropolis-Adjusted Langevin Algorithm are very popular tools for Bayesian inference on, respectively, high- and moderately high-dimensional targets. The efficiency improvements, however, come at a price. The performance of both algorithms can degrade rapidly, sometimes terminally, in the presence of large gradients; furthermore, even when the gradients are controlled, the efficiency of HMC is notoriously sensitive to the choice of tuning parameters. This session showcases new gradient-based Markov chain Monte Carlo algorithms, as well as analyses and further developments of recent innovations, that tackle these sensitivities and enable straightforward, robust, gradient-based inference.

Tuesday, July 19, 2022, 10:30 – 12:30, Lecture Hall 4

Simulation and Monte Carlo Methods in Quantitative Finance and Insurance

Organizer:

Sascha Desmettre
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Session Description:

Due to the lack of closed-form solutions, the realistic modeling of finance and insurance products requires Monte Carlo methods and sophisticated simulation methods in many cases. Areas of application include, but are not limited to, option pricing, risk assessment, the valuation of financial and insurance portfolios, portfolio optimization, the simulation of life and non-life insurance claims, death probalities, rare event simulation, etc.

This special session shall give a broad insight into some recent developments within the area of Simulation and (Quasi-) Monte Carlo Methods for Quantitative Finance and Insurance. The focus lies on problems that arise in real-world applications, for which the (Quasi-) Monte Carlo method or other simulation methods are used.

Thursday, July 21, 2022, 16:30 – 18:30, Lecture Hall 5

Smoothing and Adaptive Methods

Organizers:

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Florian Puchhammer
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Session Description:

High-dimensional problems involving singularities or discontinuities occur in many application areas, ranging from finance to uncertainty quantification. Yet, due to the resulting lack of smoothness, most computational methods for tackling high-dimensional problems break down in the presence of such singularities and discontinuities.

This special session will present recent results on how different smoothing and adaptive strategies can be employed within Monte Carlo/multilevel Monte Carlo, quasi-Monte Carlo, and similar sampling methods in order to tackle problems that lack the necessary smoothness that is typically required. Topics to be discussed by speakers in this session include methods for density estimation and rare-event simulation, as well as how smoothing and adaptivity can be used for applications such as option pricing in computational finance and uncertainty quantification. Both practical methods and theoretical results will be presented.

Part 1	Thursday, July 21, 2022, 16:30 – 18:30, Lecture Hall 1

Alexander D. Gilbert
Theory and construction of lattice rules after preintegration for pricing Asian options p. 118

Abdul-Lateef Haji-Ali
Multilevel path branching for digital options p. 126

Sebastian Krumscheid
Adaptive stratified sampling for non-smooth problems p. 141

Sifan Liu
Pre-integration via active subspaces p. 148

Part 2	Friday, July 22, 2022, 09:00 – 10:30, Lecture Hall 1

Andrea Scaglioni
Convergence of adaptive stochastic collocation with finite elements p. 193

Abirami Srikumar
Approximating distribution functions in uncertainty quantification using quasi-Monte Carlo methods p. 206

Stochastic Computation and Complexity: Approximation of SDEs with Non-standard Coefficients

Organizer:

Larisa Yaroslavtseva
University of Passau
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Session Description:

We are concerned with algorithms and complexity for computational problems of stochastic analysis, stochastic processes, high and infinite dimensional problems of analysis. This includes aspects of efficiency, optimality, lower bounds, and connections to functional analysis.

This session is devoted to the numerical analysis of SDEs with coefficients that do not satisfy the classical Lipschitz assumptions. This includes e.g. upper and lower error bounds for pathwise approximation of such SDEs as well asnew techniques from stochastic analysis to cope with the lack of regularity of the coefficients.

Part 1	Wednesday, July 20, 2022, 10:30 – 12:30, Lecture Hall 1

Andreas Neuenkirch
Optimal approximation of stochastic volatility models at a single point p. 163

Máté Gerencsér
Approximation of Lévy-driven SDEs p. 117

Konstantinos Dareiotis
Approximation of stochastic PDEs with measurable reaction term p. 104

Christopher Rauhögger
On the performance of the Euler-Maruyama scheme for multidimensional SDEs with discontinuous drift coefficient p. 179

Part 2	Thursday, July 21, 2022, 10:30 – 12:30, Lecture Hall 1

Michaela Szölgyenyi
Existence, uniqueness, and approximation for jump-driven SDEs with discontinuous drift p. 213

Chengcheng Ling
Taming singular SDEs: A numerical method p. 147

Paweł Przybyłowicz
Strong and weak approximation of solutions of SDEs under noisy information about coefficients and driving Wiener process p. 175

Kathrin Spendier
Convergence of the tamed Euler–Maruyama method for SDEs with discontinuous and polynomially growing drift p. 203

Stochastic Computation and Complexity: High Dimensional Approximation, Integration, and PDEs

Organizer:

Stefan Heinrich
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Session Description:

We are concerned with algorithms and complexity for computational problems of stochastic analysis, stochastic processes, high and infinite dimensional problems of analysis. This includes aspects of efficiency, optimality, lower bounds, and connections to functional analysis.

This session is devoted, in particular, to high dimensional approximation, integration, ODEs and PDEs.

Part 1	Tuesday, July 19, 2022, 10:30 – 12:30, Lecture Hall 1

Part 2	Tuesday, July 19, 2022, 16:30 – 18:30, Lecture Hall 1

Stochastic Computation and Complexity: Quadrature for SDEs and SPDEs, Stochastic Optimization, Neural Networks

Organizer:

Thomas Müller-Gronbach
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Session Description:

We are concerned with algorithms and complexity for computational problems of stochastic analysis, stochastic processes, high and infinite dimensional problems of analysis. This includes aspects of efficiency, optimality, lower bounds, and connections to functional analysis.

This session is devoted, in particular, to recent results in the error analysis of quadrature algorithms for S(P)DEs, stochastic approximation algorithms and deep neural networks and the interplay between these fields.

Part 1	Monday, July 18, 2022, 10:30 – 12:00, Lecture Hall 1

Part 2	Monday, July 18, 2022, 16:30 – 17:30, Lecture Hall 1

Variance Reduction Techniques for Rare Events

Organizers:

Nadhir Ben Rached
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Raúl Tempone
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Session Description:

Rare events are events with small probabilities, but their occurrences are critical in many real-life applications. The problem of estimating rare event probabilities is encountered in various engineering applications (finance, wireless communications, system reliability, Biology, etc.). Naive Monte Carlo simulations are, in this case, substantially expensive. This session focuses on methods belonging to the class of variance reduction techniques. These alternative methods deliver, when appropriately used, accurate estimates with a substantial amount of variance reduction compared to the naive Monte Carlo estimator.

Tuesday, July 19, 2022, 16:30 – 18:30, Lecture Hall 5

Nadhir Ben Rached
Efficient importance sampling algorithm applied to the performance analysis of wireless communication systems estimation p. 89

Shyam Mohan
Importance sampling methods for McKean-Vlasov type stochastic differential equations p. 159

Kemal Dinçer Dingeç
Variance reduction techniques for right-tail probabilities of exchangeable lognormal sums p. 107

Karthyek Murthy
Achieving efficiency in black-box simulation of distribution tails with self-structuring importance samplers p. 161

What Did You Expect? Equidistribution in Number Theory

Organizer:

Christoph Aistleitner
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Session Description:

The intimate connection between equidistribution and number theory goes back to Hermann Weyl's seminal work of 1916. Some of the most important topics in this context are pseudorandomness, normality, continued fractions, distributional properties of primes and other arithmetic sequences, exponential sums and metric number theory, and there are close connections with mathematical disciplines such as Diophantine approximation, harmonic analysis, ergodic theory and probability, as well as with theoretical physics. The talks in this session will focus on some of these aspects at the interface of equidistribution and number theory, and present some of the recent research topics of the number theory group at Graz University of Technology / Austria.

Wednesday, July 20, 2022, 10:30 – 12:30, Lecture Hall 3

Abstracts

Monday, July 18, 2022, 15:30 – 16:00, Lecture Hall 4

Importance Markov chain

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The Importance Markov chain is a new algorithm bridging the gap between rejection sampling and importance sampling, moving from one to the other using a tuning parameter. Based on a modified sample of an auxiliary Markov chain targeting an auxiliary target (typically with a MCMC kernel), the Importance Markov chain amounts to construct a new extended Markov chain where the marginal distribution of the first component converges to the target distribution. We obtained the geometric ergodicity for this extended kernel, under mild assumptions on the auxiliary kernel. As a typical example, the auxiliary target can be chosen as a tempered version of the target, and the algorithm then allows to explore more easily multimodal distributions. A Law of Large Numbers and a Central limit theorem are also obtained. Computationally, the algorithm is easy to implement and can use preexisting librairies to simulate the auxiliary chain.

Friday, July 22, 2022, 09:00 – 09:30, Lecture Hall 5

Linear complexity of some sequences derived from hyperelliptic curves of genus 2

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Coauthor(s): László Mérai

Special session: Pseudo-Random Number Generation p.65

In this talk, we investigate the level of randomness of specific sequences derived from hyperelliptic curves of genus 2. For elliptic curves, the randomness properties of such sequences are well-studied. Here we study the corresponding construction in the hyperelliptic case.

Let C be a hyperelliptic curve of genus 2 defined by

$$C: \; y^2 = x^5 + b_1x^4 + b_2x^3 + b_3x^2 + b_4x + b_5$$

over a finite field $\mathbb{F}_q$ of odd characteristic. One can define a group operation on the *Jacobian* J_C of the curve C. For curves of genus 2, the Jacobian is a 2 dimensional abelian variety.

We look at two different ways of generating sequences on the Jacobian, that is, the linear congruential generator and the Frobenius endomorphism generator. We show that these sequences posses good pseudorandom properties in term of linear complexity.

Our method uses an embedding of the Jacobian J_C into $\mathbb{P}^8$ provided by David Grant, which gives explicit addition formulas for points on the Jacobian. After tailoring these formulas for the Jacobian over finite fields, we are able to prove the required degree estimates in order to use Stepanov's method.

Thursday, July 21, 2022, 11:00 – 11:30, Lecture Hall 3

Constructive subsampling of finite frames with applications in optimal function recovery

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Coauthor(s): Martin Schäfer, Tino Ullrich

Special session: Approximation from Random Data p.54

In this talk we present new constructive methods, random and deterministic, for the efficient subsampling of finite frames in $\mathbb{C}^m$. Based on a suitable random subsampling strategy, we are able to extract from any given frame with bounds $0 < A \leq B < \infty$ (and condition B/A) a similarly conditioned reweighted subframe consisting of merely $\mathcal{O}(m \log m)$ elements. Further, utilizing a deterministic subsampling method based on principles developed by Batson, Spielman and Srivastava, we are able to reduce the number of elements to $\mathcal{O}(m)$ (with a constant close to one). By controlling the weights via a preconditioning step, we can, in addition, preserve the lower frame bound in the unweighted case. This allows to derive new quasi-optimal unweighted (left) Marcinkiewicz-Zygmund inequalities for $L_2(D, \nu)$ with constructible node sets of size $\mathcal{O}(m)$ for m-dimensional subspaces of bounded functions. Those can be applied e.g. for (plain) least-squares sampling reconstruction of functions, where we obtain new quasi-optimal results avoiding the Kadison-Singer theorem. Numerical experiments indicate the applicability of our results.

Tuesday, July 19, 2022, 16:30 – 17:00, Lecture Hall 3

Energy measures in Grassmannian spaces

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Coauthor(s): Diego Cuevas, Ignacio Santamaría, Vít Tuček, Gunnar Peters

Special session: Energy-Minimizing Point Configurations and Measures II p.59

Recall that the Grassmannian $\mathbb{G}(M, \mathbb{K}^T)$ is the set of M–dimensional subspaces of $\mathbb{K}^T$ where $\mathbb{K} = \mathbb{R}$ or $\mathbb{C}$ and $M < T$.

Among the many ways to define the energy of a finite collection of elements $X_1, \ldots, X_K \in \mathbb{G}(M, \mathbb{K}^T)$, one of particular interest for the so called non–coherent MIMO communication networks is given by the formula:

$$\sum_{k \neq j} \det(\mathrm{Id}_M - X_k^H X_j X_j^H X_k)^{-N},$$

for different values of N. In this talk I will describe theoretical and practical advances both in the study of lower and upper bounds for this energy and related concepts, and in the generation of actual structured and unstructured collections of points with quasioptimal energy.

This work is based in papers [1] and [2] and partially supported by grants PID2020-113887GB-I00 and PID2019-104958RB-C43 funded by MCIN/ AEI /10.13039/501100011033, as well as by project GRASSCOM, Huawei Technologies, Sweden.

[1] A Fast Algorithm for Designing Grassmannian Constellations. Diego Cuevas, Carlos Beltrán Ignacio Santamaría, Vít Tuček and Gunnar Peters. WSA 2021, EURECOM, ISBN 978-3-8007-5686-5.

[2] Union Bound Minimization Approach for Designing Grassmannian Constellations. Diego Cuevas, Carlos Beltrán Ignacio Santamaría, Vít Tuček and Gunnar Peters. To appear.

Wednesday, July 20, 2022, 14:00 – 14:30, Lecture Hall 5

Quasi-Monte Carlo and multilevel Monte Carlo combined with numerical smoothing for robust and efficient option pricing and density estimation

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In several applications, when approximating the expectation of a functional of a stochastic process, the robustness and performance of deterministic quadrature, quasi-Monte Carlo (QMC), and multilevel Monte Carlo (MLMC) methods may critically depend on the regularity of the integrand. To overcome this issue and reveal the available regularity, we consider cases in which analytic smoothing cannot be performed. In [1], we introduce a novel numerical smoothing approach by combining a root-finding algorithm with one-dimensional integration with respect to a single well-selected variable. We prove that, under appropriate conditions, the resulting function of the remaining variables is highly smooth, potentially affording the improved efficiency and robustness of QMC and MLMC methods. Our study is motivated by option pricing and density estimation problems, and our focus is on dynamics where the discretization of the asset price is necessary. Our analysis and numerical experiments in [1] demonstrate the advantages of combining numerical smoothing with the adaptive sparse grid quadrature (ASGQ) and QMC methods over ASGQ and QMC methods without smoothing. In [2], our analysis and numerical experiments show that our numerical smoothing improves the robustness (by controlling the kurtosis at deep levels) and complexity of the MLMC method. In particular, the smoothness theorem presented in [1] enables us to recover the MLMC complexities obtained for smooth or Lipschitz functionals. Moreover, our approach efficiently estimates density functions, a task that previous methods based on Monte Carlo or MLMC fail to achieve efficiently, at least in moderate to high dimensions. Finally, our approach in [1,2] is generic and can be applied to solve a broad class of problems, particularly for approximating distribution functions, financial Greeks computation, and risk estimation.

[1] Bayer, Christian, Chiheb Ben Hammouda, and Raúl Tempone. "Numerical Smoothing with Hierarchical Adaptive Sparse Grids and Quasi-Monte Carlo Methods for Efficient Option Pricing." arXiv preprint arXiv:2111.01874 (2021).

[2] Bayer, Christian, Chiheb Ben Hammouda, and Raúl Tempone. "Multilevel Monte Carlo Combined with Numerical Smoothing for Robust and Efficient Option Pricing and Density Estimation." To appear (2022).

Tuesday, July 19, 2022, 16:30 – 17:00, Lecture Hall 5

Efficient importance sampling algorithm applied to the performance analysis of wireless communication systems estimation

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Special session: Variance Reduction Techniques for Rare Events p.80

When assessing the performance of wireless communication systems operating over fading channels, one often encounters the problem of computing expectations of some functional of sums of independent random variables (RVs). The outage probability (OP) at the output of Equal Gain Combining and Maximum Ratio Combining receivers is among the most important performance metrics that falls within this framework. In general, closed form expressions of expectations of functionals applied to sums of RVs are out of reach. A naive Monte Carlo simulation is of course an alternative approach. However, this method requires a large number of samples for rare event problems (small OP values for instance). Therefore, it is of paramount importance to use variance reduction techniques to develop fast and efficient estimation methods. In this work, we use importance sampling (IS), being known for its efficiency in requiring less computations for achieving the same accuracy requirement. In this line, we propose a state-dependent IS scheme based on a stochastic optimal control formulation to calculate rare events quantities that could be written in a form of an expectation of some functional of sums of independent RVs. Our proposed algorithm is generic and can be applicable without any restriction on the univariate distributions of the different fading envelops/gains or on the functional that is applied to the sum. We apply our approach to the Log-Normal distribution to compute the OP at the output of diversity receivers with and without co-channel interference. For each case, we show numerically that the proposed state-dependent IS algorithm compares favorably to most of the well-known estimators dealing with similar problems.

Monday, July 18, 2022, 15:30 – 16:00, Lecture Hall 5

PDDSparse: a highly scalable algorithm for large-scale PDEs

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I will present a new probabilistic domain decomposition method [1]—called PDDSparse—intended for the solution of large-scale PDEs on parallel computers. The idea is to first solve the PDE along the subdomain interfaces with Feynman-Kac-based Monte Carlo simulations, thus rendering the subdomain-restricted PDEs well posed. The new insight of PDDSparse is to integrate the Feynman-Kac diffusions in the subdomains only, by coupling the unknown boundary conditions by interpolation. In this way, a stochastic linear system arises whose solution are the interfacial nodal values. This system is only $\mathcal{O}(\sqrt{N})$ (where N is the total size of the PDE discretisation), highly structured and sparse, and apparently stable. On the other hand, the Feynman-Kac diffusions are orders of magnitude faster and take only local information of the PDE for integration, while variance reduction can be incorporated naturally [2]. Preliminary results obtained in the supercomputing facility CINECA will be discussed.

[1] J.A. Acebrón, M.P. Busico, P. Lanucara, R. Spigler (2005). Domain decomposition solution of elliptic problems via probabilistic methods, SIAM J. Sci. Comput. 27, 440-457

[2] F. Bernal, and J.A. Acebrón (2016). A multigrid-like algorithm for probabilistic domain decomposition. Computers and Mathematics with Applications 72, 1790-1810.

Tuesday, July 19, 2022, 12:00 – 12:30, Lecture Hall 6

Higher order approximations of piecewise deterministic Markov processes with splitting schemes

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Special session: Recent Advances in Piecewise Deterministic Monte Carlo Methods p.71

Piecewise deterministic Markov processes (PDMPs) received substantial interest in recent years as an alternative to classical Markov chain Monte Carlo algorithms. While theoretical properties of PDMPs have been studied extensively, their practical implementation remains limited to specific applications in which bounds on the gradient of the negative log-target can be derived. In order to address this problem, we propose to approximate PDMPs using splitting schemes, that means simulating the deterministic dynamics and the random jumps in two different stages. First, we show that, as expected, basic symmetric splittings of PDMPs are of second order. Then we focus on the Zig-Zag sampler and the Bouncy Particle sampler and discuss the convergence properties of the approximations obtained using different splitting schemes. For this we study both the bias introduced by the discretisation and the rate of convergence. Numerical experiments are given to support our theoretical findings.

Thursday, July 21, 2022, 16:30 – 17:00, Lecture Hall 4

A-posteriori numerical methods for random elliptic PDEs

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Special session: Multilevel and Higher-Order Approximations for Stochastic Processes, Random Fields and PDEs p.63

Flow through fractured porous media may be modeled mathematically by partial differential equations (PDEs) with discontinuous coefficients. The spatial discontinuities in the coefficients introduce low regularity in the respective PDE solution, which in turn yields deteriorated convergence rates for standard numerical spatial discretziations. Including uncertainties representing measurement errors or unknown geometry into the model results in a random PDE, where we are interested in the efficient approximation of moments of the random PDE solution. However, the deteriorated spatial convergence rates are transferred over to the approximation of moments. In this talk we consider the application of a-posteriori error estimation techniques yielding improved spatial convergence rates, to the approximation of moments of solutions to a linear random elliptic PDE with discontinuous diffusion coefficient.

Monday, July 18, 2022, 17:00 – 17:30, Lecture Hall 3

Minimality results for the Embedded-atom model

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Special session: Periodic Point Configurations and Lattice Point Interactions p.64

The Embedded-atom model (EAM) provides a phenomenological description of atomic arrangements in metallic systems and is widely used in molecular simulations. It consists of a configurational energy depending on atomic positions and featuring the interplay of two-body atomic interactions and nonlocal effects due to the corresponding electronic clouds. In this talk, I will present minimality results for this system among lattices in dimensions 2 and 3 as well as other aspects of the problem (dilute system, equilibrium measure, etc., according to progresses made on the problem by the conference). Rigorous results based on variational arguments as well as numerics will be presented.

Tuesday, July 19, 2022, 17:30 – 18:00, Lecture Hall 1

On the properties of randomized Euler and Runge-Kutta schemes for ODEs

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Special session: Stochastic Computation and Complexity: High Dimensional Approximation, Integration, and PDEs p.78

We will report the results concerning error bounds and optimality of randomized explicit and implicit Euler schemes and the randomized two-stage Runge-Kutta scheme under inexact information and mild assumptions about the right-hand side function (including local Hölder and Lipschitz continuity in time and space variables, respectively). This part will be based on papers [2,3] which extend the well-known results for exact information and global assumptions.

Moreover, we will establish an upper bound for the probability of the exceptional set for investigated algorithms, also in the setting of inexact information, cf. [1].

[1] T. Bochacik, On the properties of the exceptional set for the randomized Euler and Runge-Kutta schemes (2022), arXiv:2202.01683.

[2] T. Bochacik, M. Goćwin, P. M. Morkisz, P. Przybyłowicz, Randomized Runge-Kutta method – Stability and convergence under inexact information, *J. Complex.* **65** (2021), 101554.

[3] T. Bochacik, P. Przybyłowicz, On the randomized Euler schemes for ODEs under inexact information (2021), arXiv:2104.15071.

Wednesday, July 20, 2022, 10:30 – 11:00, Lecture Hall 3

The L^2 discrepancy of lattices revisited

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Special session: What Did You Expect? Equidistribution in Number Theory p.81

The first N-element point set in the unit square whose L^2 discrepancy is of optimal order $\ll \sqrt{\log N}$ was found by Davenport, who constructed a symmetrized lattice using a badly approximable irrational. Revisiting this classical construction, with or without symmetrization, and using arbitrary irrationals, we established the precise relationship between the L^2 discrepancy of such lattices and the continued fraction expansion of the irrational. For instance, Davenport's construction is optimal if and only if the quadratic mean of the partial quotients is bounded; for the same construction without symmetrization to be optimal, we also need at least square root cancellation in the alternating sum of the partial quotients. We find the asymptotics for classical numbers such as quadratic irrationals or Euler's number, and also for typical irrationals by finding the limit distribution of the L^2 discrepancy. The case of rational lattices is entirely analogous, and lead to the limit distribution of the L^2 discrepancy of a randomly chosen symmetrized rational lattice.

Monday, July 18, 2022, 16:30 – 17:00, Lecture Hall 3

Lattice points to the sphere: towards discrepancy estimates

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Special session: Periodic Point Configurations and Lattice Point Interactions p.64

It is a well-known fact that an N-point configuration on the unit sphere in $\mathbb{R}^3$ that maximizes the sum of all mutual Euclidean distances has minimal spherical cap $\mathbb{L}_2$-discrepancy (Stolarsky's Invariance Principle).

Bounds for the maximal sum of distances show that this discrepancy tends to 0 as $N \to \infty$ with convergence rate $N^{-\frac{3}{4}}$. The precise asymptotic behavior is closely related to unresolved questions about the asymptotic expansion of optimal Riesz s-energy and, in turn, universal optimality of planar configuration in the context of best-packing, renormalized energy, and the optimality of the hexagonal lattice.

For constructible point sets on the sphere less is known.

Using the area-preserving Lambert cylindrical equal-area projection, a planar configuration like a (rational) lattice can be mapped to the sphere.

The so far best possible provable bound for the $\mathbb{L}_2$-discrepancy is the same as for the expected value for i.i.d. random points from 2012 for which the rate of convergence is $N^{-\frac{1}{2}}$.

In this talk, we present recent (partial) results for the Fibonacci lattice mapped to the sphere and comment on hyperuniformity of such configurations.

Wednesday, July 20, 2022, 10:30 – 11:00, Lecture Hall 6

Spectral analysis of multivariate multilevel Monte Carlo methods

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Multi-fidelity variance reduction methods are being used increasingly in different fields as an improvement over the simple Monte Carlo method. In most cases, they are used to estimate scalar quantities of interest. However, in some applications, the quantity of interest may be a statistic of a multivariate random variable, for example the expectation of a discretized random field in geosciences. In such cases, a scalar measure of the multivariate error only provides limited information, while a more thorough analysis may give better insight into the underlying error field.
This work focuses on multilevel Monte Carlo (MLMC) methods, which aim to reduce the sampling error of estimators by combining samples of different resolutions. We conduct a Fourier analysis of the error of those MLMC estimators to study the estimation quality at different scales. The conclusions allow us to improve the existing method for multivariate applications. Similar to multigrid techniques, we apply pre- and post-smoothing filters to better preserve the correlation between the different fidelity levels. This leads to a reduction of the overall estimation error along with the possibility of focusing the estimation on specific scales of interest.
The first part of the presentation introduces MLMC methods for the estimation of multivariate quantities of interest. We then present a theoretical spectral analysis for the MLMC estimation of the expectation of a discretized random field, whose conclusions motivate the introduction of filtering. Finally, we test the resulting methodology on the estimation of the diagonal of diffusion-based covariance matrices of 2D random fields.

This project has received financial support from the CNRS through the 80 | Prime program. This work was supported by the French national program LEFE (Les Enveloppes Fluides et l'Environnement).

Tuesday, July 19, 2022, 11:00 – 11:30, Lecture Hall 4

Approximate manifold sampling via the Hug sampler

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Special session: Robust Innovations in Gradient-Based MCMC p.73

Sampling from a probability density constrained to a manifold is of importance in numerous applications arising in statistical physics, statistics or machine learning. Sampling from such constrained densities, in particular using an MCMC approach, poses significant challenges and it is only recently that correct solutions have been proposed. The resulting algorithms can however be computationally expensive. We propose a relaxation of the problem where the support constraint is replaced with that of sampling from a small neighbourhood of the manifold. We develop a family of bespoke and efficient algorithms adapted to this problem and demonstrate empirically their computational superiority, which comes at the expense of a modest bias.

[1] Ludkin, M. and Sherlock, C. Hug and hop: a discrete-time, non-reversible markov chain monte-carlo algorithm, 2021.
[2] Au, K. X., Graham, M. M., and Thiery, A. H. Manifold lifting: scaling mcmc to the vanishing noise regime, 2021.
[3] Lelievre, T., Rousset, M., and Stoltz, G. Hybrid monte carlo methods for sampling probability measures on submanifolds, 2019.

Monday, July 18, 2022, 16:00 – 16:30, Lecture Hall 4

Adaptive stochastic gradient descent for Bayesian optimal experimental design

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Coauthor(s): Joakim Beck, Raúl Tempone

Experiments play a central role in many fields of science. Usually, it is of the interest of the investigators to perform experiments as efficiently as possible. However, finding the optimal design for an experiment can be a cumbersome task. In the field of Bayesian optimal experimental design, it is usual to use the mutual information between experimental observations and parameters of interest, the Expected Information Gain (EIG), as a measure of the quality of an experiment. Thus, in a gradient-based optimization approach to maximize the EIG, one needs to compute the gradient of the EIG every iteration. Here, we propose the use of an adaptive Stochastic Gradient Descent (SGD) using a double-loop Monte Carlo (DLMC) estimator of the gradient of the EIG. Every optimization iteration, we compute the DLMC sample sizes necessary to keep the relative statistical error and the relative bias uniformly bounded. Under the assumption of strong-convexity of the EIG, we prove that our method attains linear convergence iteration-wise in the L^2 sense. Our error analysis of the DLMC estimator of the gradient of the EIG incorporates discretization errors of the model, thus being suited for cases where the experiment is described by a partial or ordinary differential equation. The performance of SGD with our DLMC estimator is validated with numerical results.

Wednesday, July 20, 2022, 11:00 – 11:30, Lecture Hall 5

Adaptive reduced order models for rare event simulation

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Special session: Approximate Models for Rare Event Simulation and Uncertainty Quantification p.53

We want to compute the probability of a rare event of the form $P(S(X) > L)$, with X a random vector in $\mathbf{R}^d$, with a computable density (up to a normalization constant), and S a real function that is very expensive to compute. We assume that we have a budget, i.e., a fixed number of complete evaluations of S, and that we can also build reduced-order models of S, which can be iteratively refined when new values of S are computed. We propose a fully adaptive algorithm to iteratively build an importance sampling distribution and draw from it, the objective being the evaluation of the probability of rare events. The importance distribution takes the form of a Gibbs measure based on the current reduced order model, with parameters adjusted to minimize the relative entropy with respect to the target rare event probability distribution. A sequential Monte-Carlo technique generates from this Gibbs measure a swarm of particles, which is used as an empirical approximation of the importance distribution. At each iteration, a sample is drawn from the current empirical measure, the exact value of S calculated, the estimate of the rare event updated, as well as the reduced order model, the Gibbs measure, and the empirical sampling distribution. After the detailed presentation of the algorithm, we will give some heuristics. Some numerical results will also illustrate its relevance.

Wednesday, July 20, 2022, 11:30 – 12:00, Lecture Hall 6

Improved efficiency of multilevel Monte Carlo for stochastic PDE through strong pairwise coupling

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Coauthor(s): Hakon Hoel, Ajay Jasra, Georgios Zouraris

Multilevel Monte Carlo (MLMC) has become an important methodology in applied mathematics for reducing the computational cost of weak approximations. For many problems, it is well-known that strong pairwise coupling of numerical solutions in the multilevel hierarchy is needed to obtain efficiency gains. In this work, we show that strong pairwise coupling indeed is also important when (MLMC) is applied to stochastic partial differential equations (SPDE) of reaction-diffusion type, as it can improve the rate of convergence and thus improve tractability. For the (MLMC) method with strong pairwise coupling that was developed and studied numerically on filtering problems in [*Chernov et al., Numer. Math., 147 (2021), 71-125*], we prove that the rate of computational efficiency is higher than for existing methods. We also provide numerical comparisons with alternative coupling ideas illustrate the importance of this feature. The comparisons are conducted on a range of SPDE, which include a linear SPDE, a stochastic reaction-diffusion equation, and stochastic Allen–Cahn equation.

Friday, July 22, 2022, 09:00 – 09:30, Lecture Hall 4

Efficient algorithms for star discrepancy subset selection

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Coauthor(s): Carola Doerr, Luís Paquete

Special session: Random Points: Generation, Quality Criteria, and Applications p.69

Low-discrepancy sequences such as Sobol' and Hammersley sequences are designed to have small discrepancy values asymptotically, when the number of points tends to infinity. In practice, applications requiring low-discrepancy points sets will only use a finite, much smaller number of points. In this talk, we introduce the Star Discrepancy Subset Selection Problem [1], which consists in choosing from a set P of n points a subset P_m of size $m \leq n$ such that the L_∞-star discrepancy of P_m is minimized. The aim of this approach is to provide point sets better tailored to practical applications. Given that the complexity of calculating the star-discrepancy is $W[1]$-hard [2], it is not surprising that we are able to show that this problem is NP-hard. We provide two algorithms, respectively based on Mixed Integer Linear Programming and Branch-and-Bound, to tackle this problem. For dimensions two and three and n not too large, our algorithms provide point sets of much smaller L_∞-star discrepancy than for point sets taken directly from usual low-discrepancy sequences. We also extend this approach to the much easier to compute L_2-star discrepancy, where we can find an analogy to an unconstrained binary quadratic programming problem, with a very weak dependency on the dimension of the point set.

[1]: Franois Clément, Carola Doerr, Luís Paquete, Star discrepancy subset selection: Problem formulation and efficient approaches for low dimensions, Journal of Complexity, Volume 70, 2022, https://doi.org/10.1016/j.jco.2022.101645.

[2]: Panos Giannopoulos, Christian Knauer, Magnus Wahlstrm, Daniel Werner, Hardness of discrepancy computation and ϵ-net verification in high dimension, Journal of Complexity, Volume 28, Issue 2, 2012, Pages 162-176, https://doi.org/10.1016/j.jco.2011.09.001.

Monday, July 18, 2022, 16:00 – 16:30, Lecture Hall 5

Optimal scaling of proximal MCMC

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Proximal MCMC is a recently proposed class of MCMC methods which uses proximity maps instead of gradients to build proposal mechanisms which can be employed for both differentiable and non-differentiable targets [1]. These methods have been shown to be stable for a wide class of targets, making them a valuable alternative to Metropolis-adjusted Langevin algorithms (MALA); and have found wide application in imaging contexts [1, 2]. The wider stability properties are obtained by building the Moreau-Yoshida envelope for the target of interest, which depends on a parameter λ.

In this work we investigate the optimal scaling problem for proximal MCMC, show that MALA is a special case of this class of algorithms and provide practical guidelines for the selection of the scale parameter and the parameter λ.

[1] M. Pereyra. Proximal Markov chain Monte Carlo algorithms. *Statistics and Computing*, 26(4):745–760, 2016

[2] A. Durmus, E. Moulines, and M. Pereyra. Efficient Bayesian computation by proximal Markov chain Monte Carlo: when Langevin meets Moreau. *SIAM Journal on Imaging Sciences*, 11(1):473506, 2018.

Monday, July 18, 2022, 16:00 – 16:30, Lecture Hall 1

Numerical approximation of solutions of delay and ordinary differential equations under nonstandard assumptions and noisy information

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The classical literature concerning problem of approximation of ODEs and DDEs solutions assume some regularity of the right-hand side function of the initial value problem, commonly Lipschitz condition. Meanwhile, it turns out that the real world applications are modeled by suitable ODEs and DDEs under nonstandard assumptions. For example, a phase change of metallic materials can be modeled by DDE with a non-Lipschitz right-hand side function, see [5, chapter 3.3] and [4,3].

The talk will be divided into two parts. Firstly, we will consider a DDE case with a multidimensional right-hand side function which is also locally Hölder continuous and fulfills one-side Lipschitz condition [1]. Then, we will sketch an ODE case with a multidimensional right-hand side function where assumptions about it are also nonstandard and we allow a presence of informational noise [2]. In the both cases we show the results concerning the upper bounds on the error of the Euler scheme applied to such ODEs or DDEs. Finally, results of numerical simulations will be presented.

[1] N. Czyżewska, P. Morkisz, P. Przybyłowicz. *Approximation of solutions of DDEs under nonstandard assumptions via Euler scheme.* 2021, arXiv:2106.03731.

[2] N. Czyżewska, P. Morkisz, P. Przybyłowicz. *Approximation of solutions of ODEs with noisy information under nonstandard assumptions via Euler scheme.* In preparation.

[3] N. Czyżewska, J. Kusiak. P. Morkisz, P. Oprocha, M. Pietrzyk, P. Przybyłowicz, Ł. Rauch and D. Szeliga. *On mathematical aspects of evolution of dislocation density in metallic materials.* 2020, arXiv:2011.08504.

[4] N. Czyżewska, J. Kusiak. P. Morkisz, P. Oprocha, M. Pietrzyk, P. Przybyłowicz, Ł. Rauch, D. Szeliga. *Prediction of Distribution of Microstructural Parameters in Metallic Materials Described by Differential Equations with Recrystallization Term.* International Journal for Multiscale Computational Engineering, **17**(3) (2019), 361-371.

[5] M. Pietrzyk, Ł. Madej, Ł. Rauch, D. Szeliga. *Computational Materials Engineering: Achieving high accuracy and efficiency in metals processing simulations.* Butterworth-Heinemann, Elsevier, Amsterdam, 2015.

Wednesday, July 20, 2022, 11:30 – 12:00, Lecture Hall 1

Approximation of stochastic PDEs with measurable reaction term

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Special session: Stochastic Computation and Complexity: Approximation of SDEs with Non-standard Coefficients p.77

In this talk we will deal with the approximation of stochastic PDEs, in spatial dimension one, of the form

$$\partial_t u = \Delta u + f(u) + \xi, \qquad u(0,x) = u_0(x), \qquad (t,x) \in [0,1] \times \mathbb{T} \tag{5.1}$$

where ξ is a space-time white noise on $[0,1] \times \mathbb{T}$ and $f : \mathbb{R} \to \mathbb{R}$. While the approximation of the solution of (5.1) has been extensively studied in the case that f is Lipschitz continuous, or at least one-sided Lipschitz, very few results were available for less regular f. In this talk we will show that the rate of convergence of the fully discrete, explicit in time, finite difference scheme is 1/2 in space and 1/4 in time, even for merely bounded, measurable f. The proof relies on the regularisation effect of the noise. To exploit and quantify this effect we use an infinite dimensional version of the stochastic sewing lemma.

Tuesday, July 19, 2022, 16:30 – 17:00, Lecture Hall 6

On quantitative Laplace-type convergence results

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Special session: Laplace Approximation and Other Model-Based Preconditioning Methods for Monte Carlo Algorithms p.61

Laplace-type results characterize the limit of sequence of measures $(\pi_\varepsilon)_{\varepsilon>0}$ with density w.r.t the Lebesgue measure $(\mathrm{d}\pi_\varepsilon/\mathrm{dLeb})(x) \propto \exp[-U(x)/\varepsilon]$ when the temperature $\varepsilon > 0$ converges to 0. If a limiting distribution π_0 exists, it concentrates on the minimizers of the potential U. Classical results require the invertibility of the Hessian of U in order to establish such asymptotics. In this work, we study the particular case of norm-like potentials U and establish quantitative bounds between π_ε and π_0 w.r.t. the Wasserstein distance of order 1 under an invertibility condition of a generalized Jacobian. One key element of our proof is the use of geometric measure theory tools such as the coarea formula. We apply our results to the study of maximum entropy models (microcanonical/macrocanonical distributions) and to the convergence of the iterates of the Stochastic Gradient Langevin Dynamics (SGLD) algorithm at low temperatures for non-convex minimization.

Monday, July 18, 2022, 10:30 – 11:00, Lecture Hall 1

Optimal shallow networks

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Special session: Stochastic Computation and Complexity: Quadrature for SDEs and SPDEs, Stochastic Optimization, Neural Networks p.79

In machine learning, a neural network architecture is associated to a parametrised family of functions, the set of possible responses. In this talk we discuss existence of minimisers in certain optimisation problems (including regression) in the case where the network consists of one hidden layer equipped with ReLU activation and an additional linear neuron. We give sufficient conditions for the existence and illustrate the role of the conditions by providing counter examples.

Thursday, July 21, 2022, 15:30 – 16:00, Lecture Hall 5

Monte Carlo simulation in the mean-field LIBOR market model

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We introduce a mean-field extension of the LIBOR market model (LMM) which preserves the basic features of the original model. This mean-field LIBOR market model (MF-LMM) is designed to reduce the probability of exploding scenarios, arising in particular in the market-consistent Monte Carlo valuation of long-term guarantees. To this end, we prove existence and uniqueness of the corresponding MF-LMM and investigate its practical aspects, including a Black's formula. Moreover, we present an extensive numerical analysis of the MF-LMM. The corresponding Monte Carlo method is based on a suitable interacting particle system which approximates the underlying mean-field equation.

References:

[1] S. Desmettre, S. Hochgerner, S. Omerovic, S. Thonhauser (2022), A Mean-Field Extension of the LIBOR Market Model, *International Journal of Theoretical and Applied Finance*, No. 25, Issue No. 01, Article No. 2250005, https://doi.org/10.1142/S0219024922500054

Thursday, July 21, 2022, 10:30 – 11:00, Lecture Hall 6

Quasi-Monte Carlo methods for stochastic Landau-Lifshitz-Gilbert equations

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Special session: Quasi-Monte Carlo Methods of High Order and Beyond p.68

Quasi-Monte Carlo methods have been successfully used in applications to partial differential equations with random coefficients. In this talk we discuss the stochastic Landau-Lifshitz Gilbert equation which can be converted to a PDE with normally distributed random coefficients. Current QMC results for log-normal random coefficients only achieve an order up to $1/N$, for uniform random coefficients higher order results are available. In this PDE, the normal random coefficients only enter in a bounded form and hence there may be hope to achieve improved rates of convergence.

Tuesday, July 19, 2022, 17:30 – 18:00, Lecture Hall 5

Variance reduction techniques for right-tail probabilities of exchangeable lognormal sums

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Special session: Variance Reduction Techniques for Rare Events p.80

The calculation of extremely small tail probabilities for certain random variables has attracted the attention of researchers in the simulation area. The simulation of tail probabilities of the sum of lognormal random variables is particularly important, since the lognormal distribution has been widely used in diverse application areas such as financial engineering and electrical engineering. Moreover, the fact that the distribution of the sum of lognormals is analytically intractable makes it necessary to use a numerical method for the estimation of tail probabilities of lognormal sums. In this talk, we present new simulation algorithms for right-tail probabilities of the sum of exchangeable lognormals.

The well-known conditional Monte Carlo (CMC) method of Asmussen & Kroese [1] has an asymptotically vanishing relative error for the right-tail probabilities of the sum of independent and identically distributed (i.i.d.) lognormal random variables. The Asmussen–Kroese (AK) estimator was extended to the more general case of non-independent and non-identical sums by Kortschak & Hashorva [2]. The extended estimator is called the modified Asmussen–Kroese (MAK) estimator. Although the AK and MAK estimators are efficient in the far tails, they do not perform well in the moderate tails for small values of the standard deviation parameter σ. Also, the MAK estimator is more complicated and slower than the AK estimator, as it requires a numerical root-finding at each replication. In this talk, we present a new and simpler extension of the AK estimator for exchangeable lognormal sums. Our new estimator is in closed-from, and its combination with importance sampling (or an additional CMC) performs better than the MAK estimator for all exchangeable lognormal vectors with any correlation value and for small and large σ values.

[1] Asmussen, S., & Kroese, D. P. (2006). Improved algorithms for rare event simulation with heavy tails. *Advances in Applied Probability*, 38(2), 545–558.

[2] Kortschak, D., & Hashorva, E. (2013). Efficient simulation of tail probabilities for sums of log-elliptical risks. *Journal of Computational and Applied Mathematics*, 247, 53–67.

Tuesday, July 19, 2022, 10:30 – 11:00, Lecture Hall 6

Infinite dimensional piecewise deterministic Markov processes

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Special session: Recent Advances in Piecewise Deterministic Monte Carlo Methods p.71

In this talk we will discuss Piecewise Deterministic Markov Processes (PDMP) in infinite dimensional spaces. Recently PDMPs have recieved a lot of attention as a continuous time algorithm for sampling problems. In such problems one of the main concerns is how the algorithm performs for very high dimensional target measures. By determining the properties of PDMP in infinite dimensional settings we gain an insight into how these processes behave as the dimension tends to infinity. In this talk I will concentrate on the Boomerang Sampler and discuss well-posedness, convergence to equilibria and finite dimensional approximation of this process.

Thursday, July 21, 2022, 11:30 – 12:00, Lecture Hall 3

Weighted least-squares approximation in expected L^2 norm

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Special session: Approximation from Random Data p.54

We investigate the problem of approximating a function u in L^2 with a linear space of functions of dimension n, using only evaluations of u at m chosen points, with m of the order of n. A first approach [2], based on weighted least-squares at i.i.d random points, provides a near-best approximation of u, but requires m of order $n \log(n)$. To reduce the sample size while preserving the quality of approximation, we need a result on sums of rank-one matrices from [4], which answers to the Kadison-Singer conjecture. The results presented here, expressed in expected L^2 norm of the approximation error, can be found in [1] and will be compared to alternative approaches [3,5,6].

[1] A. Cohen and M. Dolbeault. Optimal pointwise sampling for L^2 approximation. *Journal of Complexity*, 68, 101602, 2022.

[2] A. Cohen and G. Migliorati. Optimal weighted least squares methods. *SMAI Journal of Computational Mathematics*, 3, 181–203, 2017.

[3] D. Krieg and M. Ullrich. Function values are enough for L^2-approximation: Part II. *Journal of Complexity*, 66, 101569, 2021.

[4] A. Marcus, D. Spielman and N. Srivastava. Interlacing families II: Mixed characteristic polynomials and the Kadison-Singer problem. *Annals of Mathematics* pages 327–350, 2015.

[5] N. Nagel, M. Schäfer, and T. Ullrich. A new upper bound for sampling numbers. *Foundations of Computational Mathematics*, 1–24, 2021.

[6] V. N. Temlyakov. On optimal recovery in L^2. *Journal of Complexity*, 65, 101545, 2020.

Monday, July 18, 2022, 10:30 – 11:00, Lecture Hall 4

The Kick-Kac teleportation algorithm: boost your favorite Markov Chain Monte Carlo using Kac formula

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Special session: Developments in Markov Chain Monte Carlo p.56

In this work, we propose to target a given probability measure π by combining two Markov kernels with different invariant probability measures. In its basic form, the mechanism consists in picking up the current position and moving it according to a π-invariant Markov kernel as soon as the proposed move does not fall into a predefined region. If this is the case, then we resort to the last position in this region and move it according to another auxiliary Markov kernel before starting another excursion outside the region with the first kernel. These state dependent interactions allow to combine smoothly different dynamics that can be taylored to each region while the resulting process still targets the probability measure π thanks to an argument based on the Kac formula. Under weak conditions, we obtain the Law of Large numbers starting from any point of the state space, as a byproduct of the same property for the different implied kernels. Geometric ergodicity and Central Limit theorem are also established. Generalisations where the indicator function on the region target is replaced by an arbitrary acceptance probability are also given and allow to consider any Metropolis Hastings algorithm as a particular case of this general framework. Numerical examples, including mixture of Gaussian distributions are also provided and discussed.

Monday, July 18, 2022, 11:00 – 11:30, Lecture Hall 1

Randomized operator splitting schemes for abstract evolution equations

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Special session: Stochastic Computation and Complexity: Quadrature for SDEs and SPDEs, Stochastic Optimization, Neural Networks p.79

Abstract evolution equations are an important building block for modeling processes in physics, biology and social sciences. Moreover, optimization problems can be reformulated into evolution equations. Their applications such as machine learning, benefit from randomized optimization methods like the stochastic gradient descent method. Such a stochastic optimizer can be interpreted as a randomized operator splitting scheme. While deterministic operator splitting methods are a powerful tool in the approximation of evolution equations, a randomized version has not been studied before.

In this talk, we propose a randomized operator splitting scheme in an abstract setting and exemplify the theory by considering a randomized domain decomposition scheme.

Wednesday, July 20, 2022, 11:00 – 11:30, Lecture Hall 3

Primitive rational points on expanding horospheres: effective joint equidistribution

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Special session: What Did You Expect? Equidistribution in Number Theory. p.81

Using techniques from analytic number theory, spectral theory, geometry of numbers as well as a healthy dose of linear algebra and building on a previous work by Bingrong Huang, Min Lee and myself, wefurnish a new proof of a 2016 theorem by Einsiedler, Mozes, Shah and Shapira. That theorem concerns the equidistribution of primitive rationalpoints on certain manifolds and our proof has the added benefit of yielding a rate of convergence. It turns out to have (perhaps surprising) applications to the theory of random graphs, which I shall also discuss.

Thursday, July 21, 2022, 16:00 – 16:30, Lecture Hall 5

Numerical methods for risk functionals

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In this talk we consider numerical methods for a broad class of risk models and the computation of related risk functionals. The risk models are based on piecewise deterministic Markov processes (PDMPs), which generalize most of the classically available modeling approaches. On one hand, Feynman-Kac type representations of functionals lead to a study of partial integro-differential equations, and on the other hand, the particular Markovian structure allows for a characterization by means of integral equations. Consequently, numerical schemata based on finite-differences or QMC integration can be applied. We present some first analysis on the applicability of the respective methods and consider numerical examples. In addition, we do a comparison with the quantization technique, which is somehow established for PDMPs.

Friday, July 22, 2022, 09:30 – 10:00, Lecture Hall 4

A combined use of fibrations and determinantal point processes

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Special session: Random Points: Generation, Quality Criteria, and Applications p.69

During this talk we will explain how to make use of the internal geometric structure of the spheres of odd dimension to fairy distribute points in them.

Getting into the details: we will say that a set of points $\omega_N = \{x_1, \ldots, x_N\} \subset \mathbb{S}^d$ is well distributed if its associated discrete logarithmic or Riesz s-energy defined by

$$\mathcal{E}_{\log}(\omega_N) = -\sum_{i=1}^{N} \log ||x_i - x_j||, \qquad \mathcal{E}_s(\omega_N) = \sum_{i=1}^{N} \frac{1}{||x_i - x_j||^s} \tag{5.2}$$

is small. We will use well distributed points in $\mathbb{S}^2$ and $\mathbb{PC}^d$ and the generalized Hopf fibration $\mathbb{S}^1 \hookrightarrow \mathbb{S}^{2d+1} \to \mathbb{PC}^d$ to fairy distribute points in $\mathbb{S}^{2d+1}$. We use this technique with random point processes (determinantal point processes), see [1], for odd dimensional spheres.

[1] Carlos Beltrán and Ujué Etayo. The Projective Ensemble and Distribution of Points in Odd-Dimensional Spheres. *Constructive Approximation*, 48(1):163–182, 2018.

Thursday, July 21, 2022, 11:00 – 11:30, Lecture Hall 5

Stochastic filtering for multiscale stochastic reaction networks based on hybrid approximations

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Special session: Monte Carlo Methods and Variance Reduction Techniques for Stochastic Reaction Networks p.62

In the past few decades, the development of fluorescent technologies and microscopic techniques has greatly improved scientists' ability to observe real-time single-cell activities. In this talk, we consider the filtering problem associate with these advanced technologies, i.e., how to estimate latent dynamic states of an intracellular multiscale stochastic reaction network from time-course measurements of fluorescent reporters. A good solution to this problem can further improve scientists' ability to extract information about intracellular systems from time-course experiments.

A straightforward approach to this filtering problem is to use a particle filter where particles are generated by simulation of the full model and weighted according to observations. However, the exact simulation of the full dynamic model usually takes an impractical amount of computational time and prevents this type of particle filters from being used for real-time applications, such as transcription regulation networks. Inspired by the recent development of hybrid approximations to multiscale chemical reaction networks, we approach the filtering problem in an alternative way. We first prove that accurate solutions to the filtering problem can be constructed by solving the filtering problem for a reduced model that represents the dynamics as a hybrid process. The model reduction is based on exploiting the time-scale separations in the original network and, therefore, can greatly reduce the computational effort required to simulate the dynamics. As a result, we are able to develop efficient particle filters to solve the filtering problem for the original model by applying particle filters to the reduced model. We illustrate the accuracy and the computational efficiency of our approach using several numerical examples.

Monday, July 18, 2022, 17:30 – 18:00, Lecture Hall 3

Optimal sampling strategies in time-frequency analysis

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Special session: Periodic Point Configurations and Lattice Point Interactions p.64

Time-frequency analysis lies at the intersection of harmonic analysis, functional analysis and complex analysis, but reaches into other areas, such as analytic number theory, as well. We are concerned with optimizing spectral bounds of certain self-adjoint operators on the Hilbert space of square-integrable functions on the line. These arise from Fourier transforms which are localized using a Gaussian function. D. Gabor studied these transforms already in his pioneering work on communication theory in 1946 [4]. Similar to Shannon's work on band-limited functions, we may reconstruct a function only from its samples of the localized Fourier transforms. This leads to sampling patterns (which we always assume to be a lattice) in the plane (not on the line as in Shannon's case) as we need to consider translations (time-shifts) and modulations (frequency-shifts) of the function (signal). The optimal sampling pattern turns out to be the hexagonal lattice, which had been an open conjecture for more than 20 years. In collaboration with L. Bétermin and S. Steinerberger the author was recently able to solve the problem [1]. It turns out that the sampling problem is (more than) closely related to the problem of universal optimality [2] [3] and sphere packing and covering problems.

[1] L. Bétermin, M. Faulhuber and S. Steinerberger. A variational principle for Gaussian lattice sums. arXiv preprint: 2110.06008, (2021)

[2] H. Cohn and A. Kumar. Universally optimal distribution of points on spheres. *Journal of the American Mathematical Society* 20(1):99–148, (2007)

[3] H. Cohn, A. Kumar, S. D. Miller, D. Radchenko and M. Viazovska. Universal optimality of the E_8 and Leech lattices and interpolation formulas. *Annals of Mathematics* (to appear)

[4] D. Gabor. Theory of communication. *Journal of the Institution of Electrical Engineers-Part III: Radio and Communication Engineering* 93(26): 429-441, (1946)

Tuesday, July 19, 2022, 10:30 – 11:00, Lecture Hall 3

Spherical cap discrepancy of perturbed lattices under the Lambert projection

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Special session: Energy-Minimizing Point Configurations and Measures I p.57

Given any full rank lattice Λ and a natural number N, we regard the point set $\Lambda/N \cap (0,1)^2$ under the Lambert map to the unit sphere, and show that its spherical cap discrepancy is at most of order N, with leading coefficient given explicitly and depending on Λ only. The proof is established using a lemma that bounds the amount of intersections of certain curves with fundamental domains that tile $\mathbb{R}^2$, and even allows for local perturbations of Λ without affecting the bound, proving to be stable for numerical applications. A special case yields the smallest constant for the leading term of the cap discrepancy for deterministic algorithms up to date. The talk is based on my recent paper [1].

[1] D. Ferizović: *Spherical cap discrepancy of perturbed lattices under the Lambert projection*, https://arxiv.org/abs/2202.13894 (2022).

Wednesday, July 20, 2022, 14:00 – 14:30, Lecture Hall 3

Probabilistic discrepancy bounds for negatively dependent sequences

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In [1], Aistleitner and Weimar discussed the discrepancy of infinite-dimensional infinite u.i.d. sequences. They proved probabilistic upper bounds for the discrepancy in the form of $c\sqrt{\frac{d}{N}}$, where d is the dimension and N is the sample size. This talk aims to take a closer look at how to generalize this result to sequences which are not independent, but negatively dependent instead. In order to do this, a version of the maximal Bernstein inequality for negatively dependent sequences is proven. Moreover, bounds for bracketing numbers established by Gnewuch, Pasing and Weiss in [2] are utilized to obtain a better bound for the discrepancy.From our results numerical values for c are calculated and compared with known results for different dimensions and sample sizes. Furthermore, the theoretical results are compared to numerical boundaries obtained from Monte Carlo simulation. This is work in progress and will be accompanied by a preprint in the near future.

[1] Christoph Aistleitner and Markus Weimar. Probabilistic star discrepancy bounds for double infinite random matrices. In: J. Dick, F. Y. Kuo, G. W. Peters, I.H. Sloan (Eds.), Monte Carlo and Quasi-Monte Carlo Methods 2012, volume 65 of Springer Proceedings in Mathematics and Statistics, pages 271287. Springer, 2012.
[2] Michael Gnewuch, Hendrik Pasing and Christian Weiß. A generalized Faulhaber inequality, improved bracketing covers, and applications to discrepancy. Mathematics of Computation, 90:28732898, 2021.

Monday, July 18, 2022, 11:00 – 11:30, Lecture Hall 4

Lugsail lag windows for estimating time-average covariance matrices

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Special session: Developments in Markov Chain Monte Carlo p.56

Lag windows are commonly used in time series, econometrics, steady-state simulation, and Markov chain Monte Carlo to estimate time-average covariance matrices. In the presence of positive correlation of the underlying process, estimators of this matrix almost always exhibit significant negative bias, leading to undesirable finite-sample properties. We propose a new family of lag windows specifically designed to improve finite-sample performance by offsetting this negative bias. Any existing lag window can be adapted into a lugsail equivalent with no additional assumptions. We use these lag windows within spectral variance estimators and demonstrate its advantages in a linear regression model with autocorrelated and heteroskedastic residuals. We further employ the lugsail lag windows in weighted batch means estimators due to their computational efficiency on large simulation output. We obtain bias and variance results for these multivariate estimators and significantly weaken the mixing condition on the process. Superior finite-sample properties are illustrated in a vector autoregressive process and a Bayesian logistic regression model.

Wednesday, July 20, 2022, 11:00 – 11:30, Lecture Hall 1

Approximation of Lévy-driven SDEs

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Special session: Stochastic Computation and Complexity: Approximation of SDEs with Non-Standard Coefficients p.77

We study the strong convergence rate of the Euler scheme for SDEs driven by an additive Lévy process with exponent $\alpha \in (0, 2]$. If the coefficient is regular (say, Lipschitz), then elementary arguments show L_p convergence for any p, but with rate limited by $1/p$. Somewhat surprisingly, this defect can be overcome by techniques developed for *irregular* coefficients. With these methods we are able go well beyond the Lipschitz case and cover the optimal range of Hölder continuous coefficients for all $\alpha \in [2/3, 2]$. The rate of convergence is somewhat convoluted, but is always at least $1/2$ for all moments, Lévy exponents, and admissible Hölder regularity of coefficients.

Thursday, July 21, 2022, 16:30 – 17:00, Lecture Hall 1

Theory and construction of lattice rules after preintegration for pricing Asian options

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Special session: Smoothing and Adaptive Methods p.75

Since the 1990's it has been known that quasi-Monte Carlo (QMC) methods are extremely effective at computing the integrals required for pricing Asian options, despite the fact that the kink in the payoff function means that such problems are not smooth enough for the QMC theory to apply. A popular remedy is to first smooth the payoff by preintegration, which is a specific case of the more general method of conditional sampling. Here one first integrates the non-smooth payoff with respect a specially chosen variable (or equivalently conditions on partial information), with the result being a smooth function, but now in one dimension less. In this talk we look at pricing an Asian option in d dimensions by performing preintegration and then applying a randomly shifted lattice rule on $\mathbb{R}^{d-1}$ to the result, using the weighted space setting of Nichols & Kuo. The benefit of this approach is that it allows to choose the optimal weights for a specific Asian option problem, which in turn allows tailored randomly shifted lattice rules to be constructed using the component-by-component algorithm. We give rigorous error bounds with first-order convergence and which are explicit in the dependence on dimension. Along the way we will take a detour to highlight two interesting features of the preintegration theory. First, an equivalence between the Sobolev spaces used to analyse preintegration and the weighted spaces used to analyse randomly shifted lattice rules on $\mathbb{R}^d$. Second, the necessity of the condition that the underlying function be strictly monotone with respect to the preintegration variable.

Monday, July 18, 2022, 10:30 – 11:00, Lecture Hall 5

Progress on MATLAB and C/C++ implementations of an MLMC package

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Special session: Developments in and Applications of MCQMC Software p.55

In this talk I will outline progress in the development of MATLAB and C/C++ versions of MLMC software packages [1] implementing the algorithms and example applications described elsewhere (see [2] for example).

Due to the pandemic, progress has not been as rapid as I had hoped but I will discuss

- the range of new example applications, including an example involving the rapid generation of Poisson random variables
- a highly efficient multithreaded OpenMP C++ implementation using Intel's MKL/VSL vectorised random number generators

as well as plans for

- an asynchronous GPU implementation
- extensions to MIMC and nested MLMC

with the hope of stimulating interest from others in joint development, either of the main package(s) or example applications, during the next year while I am on sabbatical.

[1] M.B. Giles. 'Multilevel Monte Carlo methods'. *Acta Numerica*, 24:259-328, 2015.

[2] https://people.maths.ox.ac.uk/gilesm/mlmc/

Tuesday, July 19, 2022, 11:00 – 11:30, Lecture Hall 3

Optimal spherical measures approximating the uniform distribution

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Special session: Energy-Minimizing Point Configurations and Measures I p.57

Let $\mathcal{B}_t$ be the set of Borel probability measures over a unit sphere $\mathbb{S}^{d-1}$ such that for each $\mu \in \mathcal{B}_t$,

$$\int_{\mathbb{S}^{d-1}} f(x)\, d\mu(x) = \int_{\mathbb{S}^{d-1}} f(x)\, d\sigma(x),$$

for every polynomial f of degree $\leq t$, where σ is the uniform probability distribution over $\mathbb{S}^{d-1}$. In other words, measure μ approximates σ for all polynomials of degree t. Measures in $\mathcal{B}_t$ with finite support correspond to quadrature formulas of degree t. If such measures are uniform distributions over their support, they correspond to spherical t-designs.

The natural problem is, given t and d, to find the "smallest" measure in $\mathcal{B}_t$. If measures are compared by the cardinality of their support, this problem becomes the classical problem of finding minimal quadrature formulas and minimal spherical designs. In this work, we study optimal measures in $\mathcal{B}_t$ with respect to other potentials. In particular, we are interested in approximating measures μ with the minimal possible diameter of their support.

Thursday, July 21, 2022, 15:30 – 16:00, Lecture Hall 3

Hermite spaces: properties, L^2-approximation, and integration

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We consider spaces of functions of infinetely many variables that are defined with the help of the orthonormal basis of univariate Hermite polynomials of $L^2(\mathbb{R}, \mu_0)$, where μ_0 is the standard normal distribution on $\mathbb{R}$. Those spaces belong to the class of reproducing kernel Hilbert spaces of increasing smoothness and their elements are defined on proper subsets of the sequence space $\mathbb{R}^{\mathbb{N}}$. Their norms are induced by an underlying function space decomposition, namely the infinite-dimensional ANOVA decomposition. We discuss further properties of those spaces and present results on L^2-approximation and integration.
Part of the talk is based on the paper

[1] M. Gnewuch, M. Hefter, A. Hinrichs, K. Ritter, *Countable tensor products of Hermite spaces and spaces of Gaussian kernels*, Preprint, arXiv:2110.05778v2, to appear in Journal of Complexity.

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Thursday, July 21, 2022, 11:00 – 11:30, Lecture Hall 6

Construction-free median lattice rules

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Special session: Quasi-Monte Carlo Methods of High order and Beyond p.68

In this talk, we consider approximating the integral of periodic functions in weighted Korobov spaces by rank-1 lattice rules. It has been well-known that good rank-1 lattice rules achieve almost the optimal rate of convergence, which is of $O(N^{-\alpha+\varepsilon})$ for arbitrarily small $\varepsilon > 0$ with $\alpha > 1/2$ being a smoothness parameter, and that such rules can be often constructed efficiently by a fast component-by-component (CBC) algorithm. However, the standard fast CBC algorithm requires appropriate α and appropriate (special forms of) weights of Korobov space as inputs, which are generally very difficult to find for a given application. We tackle with this problem by introducing *construction-free median rank-1 lattice rules*. Our approach is inspired by [1] and works as follows:

1. draw a sample of r independent generating vectors of rank-1 lattice rules,
2. compute the integral estimate for each, and
3. approximate the integral by the median of these r estimates.

Here taking the median plays a role in filtering bad generating vectors out adaptively without any knowledge on α and weights. We can prove that our median lattice rules achieve almost the optimal order of the worst-case error with a probability that converges to 1 exponentially fast as r increases. Numerical experiments illustrate and support our theoretical findings.

[1] Z. Pan and A. B. Owen. Super-polynomial accuracy of one dimensional randomized nets using the median-of-means, November 2021. arXiv:2111.12676.

Friday, July 22, 2022, 09:30 – 10:00, Lecture Hall 5

Generating pseudorandom number sequences with Gaussian distribution

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Special session: Pseudo-Random Number Generation. p.65

Generating random noise is necessary for calibrating instruments. The properties of the noise source are critical for the performance of the instrument and the physical noise sources which are all custom made for a given frequency are usually expensive, unreliable, have short lifetimes and require stabilization. A reliable noise source which can be produced by a hardware accelerator like a FPGA (Field Programmable Gate Array) is a preferable solution in most cases, therefore random sequences coming from a random number generator are an obvious choice to use. Unfortunately, most researchers have focused in generation of uniform pseudorandom sequences, while Gaussian random number generators have received less attention than deserved [2]. In this talk, we investigate modifications of classical pseudorandom number generators for generating pseudorandom number sequences with Gaussian distribution and their application for calibrating instruments in a satellite [1].

[1] Buch, K. D., Gupta, Y., Ajith Kumar, B. (2014). Variable Correlation Digital Noise Source on FPGA - A Versatile Tool for Debugging Radio Telescope Backends. *Journal of Astronomical Instrumentation, 3* (34). https://doi.org/10.1142/S225117171450007X

[2] Malik, J. S., Hemani, A. (2016). Gaussian random number generation: A survey on hardware architectures. *ACM Computing Surveys, 49*. https://doi.org/10.1145/2980052

Tuesday, July 19, 2022, 11:00 – 11:30, Lecture Hall 6

PDMP samplers for constrained spaces and discontinuous targets

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Special session: Recent Advances in Piecewise Deterministic Monte Carlo Methods p.71

During this talk, I will formally introduce piecewise deterministic Markov processes (PDMPs) endowed with 'sticky floors', 'soft walls' and 'hard walls' which can be used for Monte Carlo simulation and allow to target efficiently a rich class of measures arising in Bayesian inference. I will motivate and illustrate the framework with several statistical applications. The class of processes presented here extends the sticky PDMP samplers introduced in [1].

[1] J. Bierkens, S. Grazzi, F. van der Meulen, and M. Schauer. Sticky PDMP samplers for sparse and local inference problems. In: *arXiv preprint arXiv:2103.08478* (2021).

Monday, July 18, 2022, 10:30 – 11:00, Lecture Hall 6

A Quasi-Monte Carlo method for estimation of eigenvalues using error balancing

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Iterative Monte Carlo methods are successfully applied for estimation of the extreme eigenvalues of large sparse matrices. Recent developments in quasi-random sequences motivated us to revisit quasi-Monte Carlo approach to eigenvalue estimation. We propose a new algorithm which combines Monte Carlo power iterations with resolvent matrix, balancing of systematic and stochastic error and new variants of randomized low discrepancy sequences. Numerical tests are presented.

Monday, July 18, 2022, 16:30 – 17:00, Lecture Hall 6

Quasi-Monte Carlo methods for optimal control problems subject to parabolic PDE constraints under uncertainty

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We study the application of a tailored quasi-Monte Carlo (QMC) method to a class of optimal control problems subject to parabolic partial differential equation (PDE) constraints under uncertainty: the state in our setting is the solution of a parabolic PDE with a random thermal diffusion coefficient, steered by a control function. To account for the presence of uncertainty in the optimal control problem, the objective function is composed with a risk measure. We focus on two risk measures, both involving high-dimensional integrals with respect to the stochastic variables: the expected value and the (nonlinear) entropic risk measure. The high-dimensional integrals are computed numerically using specially designed QMC methods, and under moderate assumptions on the input random field, the error rate is shown to be essentially linear independently of the stochastic dimension of the problem – and thereby superior to ordinary Monte Carlo methods. Numerical results are presented to assess the effectiveness of our method.

Wednesday, July 20, 2022, 10:30 – 11:00, Lecture Hall 5

Recursive estimation of a failure probability for a Lipschitz function

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Special session: Approximate Models for Rare Event Simulation and Uncertainty Quantification p.53

Let $g : \Omega = [0,1]^d \to \mathbb{R}$ denote a Lipschitz function that can be evaluated at each point, but at the price of a heavy computational time. Let X stand for a random variable with values in Ω such that one is able to simulate, at least approximately, according to the restriction of the law of X to any subset of Ω. For example, thanks to Markov chain Monte Carlo techniques, this is always possible when X admits a density that is known up to a normalizing constant. In this context, given a deterministic threshold T such that the failure probability $p := \mathbb{P}(g(X) > T)$ may be very low, our goal is to estimate the latter with a minimal number of calls to g. In this aim, building on [1], we propose a recursive and (in a certain sens) optimal algorithm that selects on the fly areas of interest and estimates their respective probabilities.

[1] A. Cohen, R. Devore, G. Petrova, and P. Wojtaszczyk. Finding the minimum of a function. Methods Appl. Anal., 20(4):365-381, 2013.

Thursday, July 21, 2022, 17:00 – 17:30, Lecture Hall 1

Multilevel path branching for digital options

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Special session: Smoothing and Adaptive Methods p.75

We propose a novel Monte Carlo-based estimator for digital options with assets modelled by a stochastic differential equation (SDE) that are solved approximately using a time-stepping scheme like Euler-Maruyama or Milstein. The new estimator is based on repeated, hierarchical path splitting [1]. Using the fact that paths of an SDE solution sharing parts of a Brownian path are conditionally independent, we show that the new estimator has animproved strong convergence rate as the size of the time-step decreases. We also show that the computational complexity of Multilevel Monte Carlo (MLMC) using the new estimator is similar to the complexity of a classical MLMC estimator when applied to smoother options. In particular, when using the Euler-Maruyama scheme, we show that the computational complexity to approximate the value of a digital option with root-mean-square error, ε, is $\mathcal{O}(\varepsilon^{-2-\nu})$ for any $\nu > 0$. This is an improvement over the computational complexity of a classical Monte Carlo estimator, $\mathcal{O}(\varepsilon^{-3})$, and a classical MLMC estimator, $\mathcal{O}(\varepsilon^{-5/2})$, when approximating the value of a digital option. Using the Milstein scheme or combining with an antithetic estimator [2] reduces the computational complexity further to the canonical complexity $\mathcal{O}(\varepsilon^{-2})$.

[1] Søren Asmussen and Peter W. Glynn. *Stochastic Simulation: Algorithms and Analysis*, volume 57. Springer New York, 2007.
[2] Michael B. Giles and Lukasz Szpruch. Antithetic multilevel Monte Carlo estimation for multi-dimensional SDEs without Lévy area simulation. *The Annals of Applied Probability*, 24(4):1585–1620, August 2014.

Wednesday, July 20, 2022, 11:00 – 11:30, Lecture Hall 6

Multilevel algorithms for L^2-approximation

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We consider L^2-approximation on reproducing kernel Hilbert spaces of functions depending on infinitely many variables. This problem has been studied in [1],[2] and [3], where the upper error bounds have been achieved by using multivariate decomposition methods (fka changing dimension algorithms). We analyze the problem for a different cost model which turns out to be favourable for multilevel algorithms. The focus of the talk will be on unrestricted linear information, where we admit the evaluations of arbitrary linear functionals. Interestingly, the analysis reveals that there is a performance gap between ANOVA and non-ANOVA spaces .

References:

[1] Wasilkowski, Grzegorz W., and H. Woniakowski. "Liberating the dimension for function approximation." *Journal of Complexity* 27 (2011): 86-110.

[2] Wasilkowski, Grzegorz W., and H. Woniakowski. "Liberating the dimension for function approximation: standard information." *Journal of Complexity* 27 (2011): 417-440.

[3] Wasilkowski, Grzegorz W. "Liberating the dimension for L_2-approximation." *Journal of Complexity* 28 (2012): 304-319.

Tuesday, July 19, 2022, 16:30 – 17:00, Lecture Hall 4

Geodesic slice sampling on the sphere

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Special session: Recent Advances in MCMC Sampling Techniques p.70

We introduce a geodesic slice sampler on the Euclidean sphere (in arbitrary but fixed dimension) that can be used for approximate sampling from distributions that have a density with respect to the corresponding surface measure. Such distributions occur e.g. in the modelling of directional data or shapes. Under some mild conditions we show that the corresponding transition kernel is well-defined, in particular, that it is reversible with respect to the distribution of interest. Moreover, if the density is bounded away from zero and infinity, then we obtain a uniform ergodicity convergence result. Finally, we illustrate the performance of the geodesic slice sampler on the sphere with numerical experiments.

Thursday, July 21, 2022, 10:30 – 11:00, Lecture Hall 4

Analysis of a localized non-linear ensemble Kalman–Bucy filter with sparse observations

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Special session: Advanced Particle Methods for Bayesian Inference p.50

With large scale availability of precise real time data, their incorporation into physically based predictive models, became increasingly important. This procedure of combining the prediction and observation is called data assimilation. One especially popular algorithm of the class of Bayesian sequential data assimilation methods is the ensemble Kalman filter which successfully extends the ideas of the Kalman filter to the non-linear situation. However, in case of spatio-temporal models one regularly relies on some version of localization, to avoid spurious oscillations.

In this work we develop a-priori error estimates for a time continuous variant of the ensemble Kalman filter, known as localized ensemble Kalman–Bucy filter. More specifically we aim for the scenario of sparse observations applied to models from fluid dynamics.

Wednesday, July 20, 2022, 11:30 – 12:00, Lecture Hall 3

On the metric theory of approximations by reduced fractions: Quantifying the Duffin-Schaeffer conjecture

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Special session: What Did You Expect? Equidistribution in Number Theory p.81

Let $\psi : \mathbb{N} \to [0, 1/2]$ be given. Koukoulopoulos and Maynard (2020) proved the Duffin–Schaeffer conjecture: for almost all reals α there are infinitely many coprime solutions (p, q) to the inequality $|\alpha - p/q| < \psi(q)/q$, if and only if the series $\sum_{q=1}^{\infty} \varphi(q)\psi(q)/q$ is divergent. In a recent joint work with Christoph Aistleitner and Bence Borda, we established a quantitative version of this result in the following sense: for almost all α, the number of coprime solutions (p, q), subject to $q \leq Q$, is of asymptotic order $\Psi(Q) = \sum_{q=1}^{Q} 2\varphi(q)\psi(q)/q$.

In this talk, I will give an overview of the original proof of Koukoulopoulos and Maynard and the additional ideas we used to obtain this quantification.

Tuesday, July 19, 2022, 18:00 – 18:30, Lecture Hall 1

A stochastic discretization method and some applications in IBC

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Special session: Stochastic Computation and Complexity: High Dimensional Approximation, Integration, and PDEs p.78

We study the complexity of problems defined on Sobolev spaces which do not satisfy the embedding condition (that is, the space is not embedded into the space of continuous functions on the corresponding domain). We consider standard information, that is, function values. Using a stochastic discretization technique, we derive new results on the complexity of integration, approximation and parametric integration in the restricted randomized setting (only random bits can be used) and in the quantum setting. For these problems the case of spaces not satisfying the embedding condition has not been considered previously in either settings. Our results also allow new comparisons between the randomized and quantum setting.

Monday, July 18, 2022, 11:30 – 12:00, Lecture Hall 5

Challenges in developing great MCQMC software

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Special session: Developments in and Applications of MCQMC Software p.55

The process of translating new Monte Carlo and Quasi-Monte Carlo (MCQMC) algorithms into software libraries faces several challenges. Great software should be easy to use with reasonable default options for the novice and advanced features for the developer or experienced user. The library architecture must allow for growth. Ensuring connectivity with other software libraries will facilitate a larger user base of the MCQMC library. Coding algorithms the right way may significantly improve their runtime or portability. Since development team members will come and go, the shared wisdom of the development team must be documented and transmitted to succeeding generations. Software developers must keep abreast of the newest computing environments to ensure peak performance. This talk will highlight some of these challenges and ways to address them.

Thursday, July 21, 2022, 16:00 – 16:30, Lecture Hall 6

An efficient estimator of nested expectations without conditional sampling

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Coauthor(s): Takashi Goda

Estimating nested expectations is an important task in computational mathematics and statistics. In our study we propose a new Monte Carlo method to estimate nested expectations efficiently without taking samples of the inner random variable from the conditional distribution given the outer random variable. This property provides the advantage over many existing methods that it enables us to estimate nested expectations only with a dataset on the pair of the inner and outer variables drawn from the joint distribution. We show an upper bound on the mean squared error of the proposed method under some assumptions. Numerical experiments are conducted to compare our proposed method with several existing methods and we see that our proposed method is superior to the compared methods in terms of efficiency and applicability.

Friday, July 22, 2022, 10:00 – 10:30, Lecture Hall 4

Consistency of randomized integration points

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Special session: Random Points: Generation, Quality Criteria, and Applications p.69

For integrable functions we present a weak law of large numbers for structured Monte Carlo methods, such as estimators based on randomized digital nets, Latin hypercube sampling, randomized Frolov point sets as well as Cranley-Patterson rotations. Moreover, median modified methods are discussed and we show that for integrands in L^p with $p > 1$ a strong law of large numbers holds.

Monday, July 18, 2022, 16:30 – 17:00, Lecture Hall 4

Wavelet frames with grid-like time-frequency sampling and quasi-random delays

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A wavelet frame consists of countably many dilated and translated copies $\psi_{a,x} = \mathbf{D}_a \mathbf{T}_\mathbf{x} \psi$ of a *mother wavelet* ψ. A *frame* is characterized by the distinctive property that any square-integrable function can be represented as a linear combination of its elements with coefficients of equivalent norm.

The study of collections $(\psi_{a_j,x_j})_{j\in J}$ which form a frame popularized frame theory in the 1980s and has remained a topic of notable interest ever since, for wavelet transforms and various constructive or abstract generalizations thereof. We revisit the original problem of finding wavelet frames for functions on the real line, and propose a new selection scheme, considering sequences $(\psi_{ak^{-1},bl+\delta_k})_{k\in\mathbb{N},l\in\mathbb{Z}}$, where $a, b > 0$, and, crucially, $\delta_k \in [0, b)$ is a quasi-random sequence. We demonstrate that, up to technicalities at very large scales, this selection scheme yields wavelet frames, provided that a, b are sufficiently small. When a digital sequence, such as the *van der Corput sequence*, is chosen for $\{\delta_k\}_{k\in\mathbb{N}}$, our proof is particularly simple. In contrast, choosing all δ_k from a fixed finite subset of $[0, b)$ will never yield a frame, independent of a, b.

Interpreting the mother wavelet as a band-pass filter, and recalling the commutation relations of dilation operators and the Fourier transform $\mathcal{F}\mathbf{D}_a = \mathbf{D}_{1/a}\mathcal{F}$, the proposed selection scheme corresponds to a regular time-frequency grid, up to the introduction of the quasi-random *delays* δ_k. In particular, if the delays δ_k are chosen according to a Kronecker sequence, then the resulting point set is a lattice. While wavelet frames with scale-dependent translation spacing must be considered in the abstract framework of generalized shift-invariant systems, our construction can draw on the rich theory of (standard) shift-invariant systems. In particular, the theoretical analysis of shift-invariant frames and the related operators is significantly easier and their implementation can rely on highly efficient algorithms.

I will present the current state of our work-in-progress investigation of shift-invariant wavelet systems with quasi-random delays on the real line, in both theoretical results and numerical studies. Finally, some indication that the proposed construction extends to an (almost) universal sampling scheme for general time-frequency systems of arbitrary dimensionality will be presented.

Monday, July 18, 2022, 11:00 – 11:30, Lecture Hall 6

Improved Bernoulli mean estimation for Monte Carlo data

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Consider the problem of estimating the mean p of a 0-1 (Bernoulli) random variable. The Gamma Bernoulli Approximation Scheme (GBAS) is an estimate with a user specified relative error distribution, that is, the distribution of the relative error is independent of p. This allows for very precise targeting of the run time to achieve any desired relative loss. GBAS operates by smoothing geometric random variables of mean $1/p$ into exponential random variables of mean $1/p$. While the benefits of using scalable exponentials versus geometric random variables are clear, this does result in the elimination of a factor of $1-p$ in the variance. This can become significant for problems where p is large. This work considers several different methods for addressing this problem. First, modifications to GBAS are considered, including the use of multiple intervals created by using antithetic and uniform shifted lattice points for turning the geometric into exponential random variables. Second, improvements to tail bounds of negative binomial random variables are considered. The result is that a significant portion of the $1-p$ factor can be retrieved while maintaining exact confidence intervals.

Wednesday, July 20, 2022, 10:30 – 11:00, Lecture Hall 4

On unbiased score estimation for partially observed diffusions

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Special session: Recent Advances in Unbiased Estimation Techniques p.72

We consider the problem of statistical inference for a class of partially observed diffusion processes, with discretely-observed data and finite-dimensional parameters. We construct unbiased estimators of the score function, i.e. the gradient of the log-likelihood function with respect to parameters, with no time-discretization bias. These estimators can be straightforwardly employed within stochastic gradient methods to perform maximum likelihood estimation or Bayesian inference. As our proposed methodology only requires access to a time-discretization scheme such as the Euler-Maruyama method, it is applicable to a wide class of diffusion processes and observation models. Our approach is based on a representation of the score as a smoothing expectation using Girsanov theorem, and a novel adaptation of the randomization schemes developed in [1], [2] and [3]. This allows one to remove the time-discretization bias and burn-in bias when computing smoothing expectations using the conditional particle filter of [4]. Central to our approach is the development of new couplings of multiple conditional particle filters. We prove under assumptions that our estimators are unbiased and have finite variance. The methodology is illustrated on several challenging applications from population ecology and neuroscience.

[1] D. Mcleish. A general method for debiasing a Monte Carlo. *Monte Carlo Methods and Applications*, 17:301315, 2011.

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[3] P. E. Jacob, F. Lindsten, and T. B. Schn. Smoothing with couplings of conditional particle filters. *Journal of the American Statistical Association*, 115(530):721729, 2020. [4] C. Andrieu, A. Doucet, and R. Holenstein. Particle Markov chain Monte Carlo methods. *Journal of the Royal Statistical Society: Series B (Statistical Methodology)*, 72(3):269342, 2010.

Monday, July 18, 2022, 17:00 – 17:30, Lecture Hall 6

Revisiting the dimension truncation error of parametric elliptic PDEs

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Elliptic PDEs with uncertain or random inputs have been considered in many studies of uncertainty quantification. In forward uncertainty quantification, one is interested in analyzing the stochastic response of the PDE subject to input uncertainty, which usually involves solving high-dimensional integrals of the PDE output over a sequence of stochastic variables. In practical computations, one typically needs to discretize the problem in several ways: approximating an infinite-dimensional input random field with a finite-dimensional random field, spatial discretization of the PDE using, e.g., finite elements, and approximating high-dimensional integrals using cubatures such as the quasi-Monte Carlo method.

In this talk, we focus on the error resulting from dimension truncation of the input random field. In particular, we demonstrate in high-dimensional problems which do not conform to the ordinary affine-parametric operator equation setting how Taylor series can be used to derive theoretical dimension truncation rates—and, in some cases, improve existing rates. Numerical examples support our theoretical findings.

Monday, July 18, 2022, 17:00 – 17:30, Lecture Hall 4

Direct simulation Monte Carlo and oscillations in aggregation-fragmentation kinetics

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Aggregation kinetics describes the interaction of colliding particle clusters that form larger agglomerates as time goes on. The evolution of cluster size densities in such systems can be efficiently computed via Monte Carlo methods. However, these algorithms experience a significant slowdown during fragmentation events due to the volume of updates for a non-constant number of new particles. In our talk we discuss how to extend two popular Direct Simulation Monte Carlo methods to aggregation processes with collisional fragmentation while preserving their efficiency [1]. We adapt underlying data structures to efficiently handle many updates at once.

To demonstrate the applicability of the approaches, we compare their performance and accuracy with efficient deterministic finite-difference method applied to the same model [2]. Additionally, we use these methods to verify the existence of oscillating regimes in the aggregation-fragmentation kinetics recently detected in deterministic simulations. We confirm that steady oscillations of densities are stable with respect to fluctuations and noise.

S. M. was supported by Russian Science Foundation (project 21-71-10072).

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[2] Matveev S. A., Krapivsky P. L., Smirnov A. P., Tyrtyshnikov E. E., & Brilliantov N. V. (2017). Oscillations in aggregation-shattering processes. Physical review letters, 119(26), 260601.

Thursday, July 21, 2022, 11:30 – 12:00, Lecture Hall 6

Density estimation in RKHS with application to Korobov spaces in high dimensions

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Special session: Quasi-Monte Carlo Methods of High Order and Beyond p.68

In this talk, we will consider a kernel method for estimating a probability density function (pdf) from an i.i.d. sample drawn from such density. Our estimator is a linear combination of kernel functions, the coefficients of which are determined by a linear equation. We will present an error analysis for the mean integrated squared error in a general reproducing kernel Hilbert space setting. Then, we will discuss how this theory can be applied to estimate pdfs for circular data. Under a suitable smoothness assumption, our method attains a rate arbitrarily close to the optimal rate.

Tuesday, July 19, 2022, 12:00 – 12:30, Lecture Hall 5

Quasi-Monte Carlo algorithms (not only) for graphics software

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Special session: Algorithmic Advancements in MCQMC Software p.51

Quasi-Monte Carlo methods are industry standard in computer graphics. We discuss fast algorithms for low discrepancy sequences and numerical traps that may be encountered in practice. We take a fresh look at massively parallel quasi-Monte Carlo integro-approximation for the purpose of image synthesis by light transport simulation. While being of superior uniformity, low discrepancy points may be optimized with respect to additional criteria, such as noise characteristics at low sampling rates or behavior of low-dimensional projections. Several such approaches including dimension reordering and optimization by scrambling are reviewed.

Friday, July 22, 2022, 10:30 – 11:00, Lecture Hall 4

Stratified and jittered sampling in discrepancy theory

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Special session: Random Points: Generation, Quality Criteria, and Applications p.69

We discuss properties and discrepancies of stratified samples $\mathcal{P}$ of the unit cube. More specifically, let $N \in \mathbb{N}$ be given, assume that $\Omega_1, \ldots, \Omega_N$ is a partition of $[0,1]^d \subset \mathbb{R}^d$, and let the ith random point in $\mathcal{P}$ be chosen uniformly in the ith set of the partition (and stochastically independent of the other points), $i = 1, \ldots, N$.

The first part of the talk is devoted to the question whether a partition into N sets exists such that the expected discrepancy of $\mathcal{P}$ becomes minimal. Geometric arguments reveal that this indeed is the case when the sets $\Omega_1, \ldots, \Omega_N$ are equivolume and have a reach that is bounded away from zero by a positive constant. For instance, convex sets of given volume satisfy this condition. The assumptions on the underlying discrepancy are rather weak, so the result holds in particular for the mean $\mathcal{L}_p$-discrepancy and for the star discrepancy.

In the second part, we compare mean $\mathcal{L}_p$-discrepancies for $1 \le p < \infty$ of stratified samples with one another and with the ground model of i.i.d. random points in the unit square. Generalizing a result by Pausinger & Steinerberger we show the *strong partition principle*, stating that the mean $\mathcal{L}_p$-discrepancy of a stratified sample from N equivolume sets is always strictly smaller that the mean $\mathcal{L}_p$-discrepancy of equally many i.i.d. points ('*stratification is better*'). A prominent example is jittered sampling –which can be used when $N = m^d$, $m \in \mathbb{N}$– where the sets Ω_i are all translations of $[0, 1/m]^d$. It will be shown that jittered sampling is in general not the above mentioned minimizer ('*jitter is not best*'). We will construct a partition of the unit cube into m^d convex sets of equal volume, such that the corresponding sample has a better mean $\mathcal{L}_2$-discrepancy than jittered sampling with equally many points.

Tuesday, July 19, 2022, 17:00 – 17:30, Lecture Hall 6

Stability of MAP estimation via Γ-convergence of Onsager–Machlup functionals

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Special session: Laplace Approximation and Other Model-Based Preconditioning Methods for Monte Carlo Algorithms p.61

The Bayesian solution to a statistical inverse problem can be summarised by a mode of the posterior distribution, i.e. a maximum a posteriori (MAP) estimator. The MAP estimator essentially coincides with the (regularised) variational solution to the inverse problem, seen as minimisation of the Onsager–Machlup (OM) functional of the posterior measure. An open problem in the stability analysis of inverse problems is to establish a relationship between the convergence properties of solutions obtained by the variational approach and by the Bayesian approach. To address this problem, we propose a general convergence theory for modes in [1,2] that is based on the Γ-convergence of Onsager–Machlup functionals, and apply this theory to a large class of prior distributions.

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[2] B. Ayanbayev, I. Klebanov, H. C. Lie, T. J. Sullivan, Γ-convergence of Onsager-Machlup functionals: II. Infinite product measures on Banach spaces. Inverse Problems 38 (2022), no. 2, Paper No. 025006

Tuesday, July 19, 2022, 11:00 – 11:30, Lecture Hall 1

Lower bounds for integration and recovery in L_2

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Special session: Stochastic Computation and Complexity: High Dimensional Approximation, Integration, and PDEs p.78

Function values are, in some sense, "almost as good" as general linear information for L_2-approximation (optimal recovery, data assimilation) of functions from a reproducing kernel Hilbert space. This was recently proved by new *upper bounds* on the sampling numbers under the assumption that the singular values of the embedding of this Hilbert space into L_2 are square-summable, see [2,3]. Here we mainly prove new *lower bounds*. In particular we prove that the sampling numbers behave worse than the approximation numbers for Sobolev spaces with small smoothness. Hence there can be a logarithmic gap also in the case where the singular numbers of the embedding are square-summable. We first prove new lower bounds for the integration problem, again for rather classical Sobolev spaces of periodic univariate functions.

[1] A. Hinrichs, E. Novak, D. Krieg, and J. Vybíral, Lower bounds for integration and recovery in L_2, arXiv preprint, 2021.

[2] D. Krieg and M. Ullrich, Function values are enough for L_2-approximation, *Foundations of Computational Mathematics*, 2021.

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Thursday, July 21, 2022, 17:30 – 18:00, Lecture Hall 1

Adaptive stratified sampling for non-smooth problems

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Special session: Smoothing and Adaptive Methods p.75

Various sampling methods, including the multilevel Monte Carlo method, have been established as general-purpose procedures for efficiently quantifying uncertainties in computational models. The improved computational efficiency of these sampling methods compared to vanilla Monte Carlo sampling is usually obtained by suitable variance reduction techniques. It is known, however, that these techniques may not provide performance gains when there is a non-smooth, in particular discontinuous, parameter dependence. Moreover, in many applications some key variance reduction ideas cannot be fully exploited, such as those of multilevel Monte Carlo, for example, when a hierarchy of computational models cannot be easily constructed. An alternative means to obtain variance reduction in these cases is offered by stratified sampling methods. In this talk, we will discuss various ideas on adaptive stratified sampling methods tailored to applications with a discontinuous parameter dependence. Examples exhibiting discontinuous solutions include hyperbolic PDEs under uncertainty, such as the Euler equations describing a high-speed flow, and the shallow water equations modeling dam breaks, flooding and atmospheric flow. For such discontinuous problems, the stochastic domain is adaptively stratified using local variance estimates, and the samples are sequentially allocated to the strata for asymptotically optimal variance reduction. The proposed methodology is demonstrated on discontinuous test cases from computational fluid mechanics and CO2 storage in subsurface reservoirs.

Tuesday, July 19, 2022, 12:00 – 12:30, Lecture Hall 1

Approximation in periodic Gevrey spaces

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Special session: Stochastic Computation and Complexity: High Dimensional Approximation, Integration, and PDEs p.78

In my talk I will first introduce periodic Gevrey spaces $G^{s,c}(\mathbb{T}^d)$, a family of Hilbert spaces closely related to Gevrey classes. More than 100 years ago these by now famous classes were defined by Maurice Gevrey, motivated by applications to PDEs.

Then the approximation numbers a_n of the embeddings $G^{s,c}(\mathbb{T}^d) \hookrightarrow L_2(\mathbb{T}^d)$ will be studied, not only the asymptotic rate, but also the behaviour in the preasymptotic range $n \leq 2^d$. Clearly, for computational aspects of high-dimensional approximation problems, it is more important to have good bounds in this range rather than to know 'only' the excat asymptotics as n tends to infinity.

If time allows I will also give an interpretation of these results in terms of tractability notions from Information-Based Complexity. Finally I will compare our new results for Gevrey embeddings with the corresponding known ones for mixed-order Sobolev embeddings.

Thursday, July 21, 2022, 18:00 – 18:30, Lecture Hall 5

Severity modeling of extreme insurance claims for tariffication

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Special session: Simulation and Monte Carlo Methods in Quantitative Finance and Insurance p.74

Generalized linear models (GLMs) are common instruments for the pricing of non-life insurance contracts. They are used to estimate the expected severity of insurance claims. We develop the threshold severity model (see [1]) that splits the claim size distribution in areas below and above a given threshold. More specifically, the extreme insurance claims above the threshold are modeled in the sense of the peaks-over-threshold (POT) methodology from extreme value theory using the generalized Pareto distribution for the excess distribution, and the claims below the threshold are captured by a GLM based on the truncated gamma distribution. To the best of our knowledge, the threshold severity model for the first time combines the POT modeling for extreme claim sizes with GLMs based on the truncated gamma distribution. We develop the corresponding log-likelihood function with respect to right-censored claim sizes, which is a typical issue that arises for instance in private or car liability insurance contracts. Finally, we demonstrate the behavior of the threshold severity model compared to the commonly used GLM based on the gamma distribution in the presence of simulated extreme claim sizes following a log-normal as well as Burr Type XII distribution.

[1] C. Laudagé, S. Desmettre & J. Wenzel (2019). Severity Modeling of Extreme Insurance Claims for Tariffication. *Insurance: Mathematics and Economics, 88*, 77-92. doi:10.1016/j.insmatheco.2019.06.002

Tuesday, July 19, 2022, 15:30 – 16:00, Lecture Hall 4

Stratified sampling for simulating multi-dimensional Markov chains

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Monte Carlo (MC) is widely used for the simulation of discrete time Markov chains. Here, N copies of the chain are simulated in parallel, using pseudorandom numbers and we extend the analysis of [1]: we consider the case of a d-dimensional continuous state space and we restrict ourselves to chains whose d components are advanced independently from each other. We replace pseudorandom numbers on $I^d := [0, 1)^d$ with stratified random points over I^{2d}: for each point, the first d components are used to select a state and the last d components are used to advance the chain by one step. We use the simple stratification technique: for $N = p^{2d}$ samples, the unit hypercube is dissected into p^{2d} hypercubes and there is one sample in each of them. The strategy outperforms usual MC if a well-chosen multivariate sort of the states is employed to order the chains at each step. We prove that the variance of the stratified sampling estimator is bounded by $\mathcal{O}(N^{-(1+1/2d)})$, while it is bounded by $\mathcal{O}(N^{-1})$ for MC. We compare these results with those of numerical experiments.

[1] El Haddad, R., El Maalouf, J., Lécot, C., L'Ecuyer,P.: Sudoku Latin square sampling for Markov chain simulation. In: B. Tuffin, P. L'Ecuyer (eds.), Monte Carlo and Quasi-Monte Carlo Methods, pp. 207–230. Springer, Cham (2020)

Monday, July 18, 2022, 11:00 – 11:30, Lecture Hall 5

An update on Lattice Tester, LatMRG, and Lattice Builder

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Special session: Developments in and Applications of MCQMC Software p.55

Lattice Tester, LatMRG, and LatNet Builder [1] are a trio of C++ libraries and programs connected to each other, whose purpose is to measure the quality of lattices in general, study the lattice structure of random number generators and search for generators with good structures, and construct good point sets and sequences for quasi-Monte Carlo. The three tools are available on GitHub and can already be used, although all three are still evolving. LatMRG and Lattice Tester were originally written in the Modula-2 language [2, 3] and have been rewritten in C++, although not yet completely. Both LatMRG and LatNet Builder use Lattice Tester.

In this talk, we will provide a summary of what these tools are doing, an update of their status, and what they should offer in the near future. For the latter, we will also be happy to receive suggestions from the session participants.

[1] P. L'Ecuyer, P. Marion, M. Godin, and F. Puchhammer, "A Tool for Custom Construction of QMC and RQMC Point Sets," Monte Carlo and Quasi-Monte Carlo Methods 2020, A. Keller, Ed., Springer-Verlag, to appear, 2022.

[2] P. L'Ecuyer and R. Couture, "An Implementation of the Lattice and Spectral Tests for Multiple Recursive Linear Random Number Generators", INFORMS Journal on Computing, 9, 2 (1997), 206–217.

[3] P. L'Ecuyer and R. Couture, "LatMRG Users Guide: A Modula-2 software for the theoretical analysis of linear congruential and multiple recursive random number generators", https://www-labs.iro.umontreal.ca/∼lecuyer/myftp/papers/guide-latmrg-m2.pdf, 2000.

[4] The three GitHub pages can be found at https://github.com/umontreal-simul.

Friday, July 22, 2022, 09:00 – 09:30, Lecture Hall 3

Orthogonal projection on manifolds and numerical schemes for SDEs

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Special session: Analysis and Simulation of SDEs in Non-Standard Settings p.52

In [2] and [3], numerical schemes for multidimensional stochastic differential equations (SDEs) with discontinuous drift terms and degenerate diffusions have been studies. The points of discontinuity of the drift coefficient were required to be a smooth (C^4) manifold $\Theta \subseteq \mathbb{R}^d$. On the complement of this manifold, the drift was assumed to be smooth and thus locally Lipschitz continuous.

In [3], a transform was constructed, which transforms the SDE with discontinuous drift into one with Lipschitz continuous drift, thus allowing the application of classical results. This transform requires the so called unique nearest point property of the manifold Θ as well as the function which assigns the nearest point $p(x)$, i.e. the projection, to an ambient point $x \in \mathbb{R}^d \setminus \Theta$. In [1] we study for which classes of manifolds this function p exists and which regularity properties it has. This opens the way for the study of tighter conditions under which the transform method may still be applied.

[1] G. Leobacher and A. Steinicke. Exception sets of intrinsic and piecewise Lipschitz functions. *Journal of Geometric Analysis*, 32, 2022.

[2] G. Leobacher and M. Szölgyenyi. A strong order 1/2 method for multidimensional SDEs with discontinuous drift. *Ann. Appl. Probab.*, 27(4):2383–2418, 2017.

[3] G. Leobacher and M. Szölgyenyi. Convergence of the Euler-Maruyama method for multi-dimensional SDEs with discontinuous drift and degenerate diffusion coefficient. *Numerische Mathematik*, 138(1):219–239, 2018.

Thursday, July 21, 2022, 11:00 – 11:30, Lecture Hall 1

Taming singular SDEs: A numerical method

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Special session: Stochastic Computation and Complexity: Approximation of SDEs with Non-Standard Coefficients p.77

We consider a generic and explicit tamed Euler–Maruyama scheme for multidimensional time-inhomogeneous stochastic differential equations with multiplicative Brownian noise. The diffusive coefficient is uniformly elliptic, Hölder continuous and weakly differentiable in the spatial variables while the drift satisfies the Ladyzhenskaya-Prodi-Serrin condition, as considered by Krylov and Röckner (2005). In the discrete scheme, the drift is tamed by replacing it by an approximation. A strong rate of convergence of the scheme is provided in terms of the approximation error of the drift in a suitable and possibly very weak topology. A few examples of approximating drifts are discussed in detail. The parameters of the approximating drifts can vary and—under suitable conditions—be fine-tuned to achieve the standard 1/2-strong convergence rate with a logarithmic factor.

Thursday, July 21, 2022, 18:00 – 18:30, Lecture Hall 1

Pre-integration via active subspaces

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Special session: Smoothing and Adaptive Methods p.75

Pre-integration is an extension of conditional Monte Carlo to quasi-Monte Carlo and randomized quasi-Monte Carlo. It can reduce but not increase the variance in Monte Carlo. For quasi-Monte Carlo it can bring about improved regularity of the integrand with potentially greatly improved accuracy. Pre-integration is ordinarily done by integrating out one of d input variables to a function. In the common case of a Gaussian integral one can also pre-integrate over any linear combination of variables. We propose to do that and we choose the first eigenvector in an active subspace decomposition to be the pre-integrated linear combination. We find in numerical examples that this active subspace pre-integration strategy is competitive with pre-integrating the first variable in the principal components construction on the Asian option where principal components are known to be very effective. It outperforms other pre-integration methods on some basket options where there is no well established default. We show theoretically that, just as in Monte Carlo, pre-integration can reduce but not increase the variance when one uses scrambled net integration. We show that the lead eigenvector in an active subspace decomposition is closely related to the vector that maximizes a less computationally tractable criterion using a Sobol' index to find the most important linear combination of Gaussian variables. They optimize similar expectations involving the gradient. We show that the Sobol' index criterion for the leading eigenvector is invariant to the way that one chooses the remaining $d-1$ eigenvectors with which to sample the Gaussian vector.

Monday, July 18, 2022, 10:30 – 11:00, Lecture Hall 3

Lower bounds for the logarithmic energy on $\mathbb{S}^2$ and for the Green energy on $\mathbb{S}^n$

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Special session: Quantifying Notions of Equidistribution on the Sphere p.66

Smale's problems are a list of 18 challenging problems for the twenty-first century proposed by Field's medallist Steve Smale. The 7th problem is to give a simple and efficient description, or alternatively describe an algorithm, to place N points in the sphere such that their logarithmic potential is very close to the minimum. A major difficulty in this problem is that the value of the minimal logarithmic energy on the sphere is not fully known. The current knowledge is:

$$\kappa N^2 - \frac{1}{2} N \ln N + C_{\log} N + o(N),$$

where κ is the continuous energy and $C_{\log}$ is a constant such that

$$-0.0568\ldots = \ln 2 - \frac{3}{4} \leqslant C_{\log} \leqslant 2\ln 2 + \frac{1}{2}\ln\frac{2}{3} + 3\ln\frac{\sqrt{\pi}}{\Gamma(1/3)} = -0.0556\ldots,$$

where the lower bound $-0.0568\ldots$ was proved by Lauritsen building upon previous results by Sandier, Serfaty and Betermin. In fact, the upper bound has been conjectured to be an equality and it is one of the most important open problems in the area. In the talk I will show an alternative proof of Lauritsen's lower bound for the constant $C_{\log}$. This new approach generalizes to new lower bounds for the Green energy of $\mathbb{S}^n$.

References

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2. Lauritsen, A. B. (2021) *Floating Wigner crystal and periodic jellium configurations.* J. Math. Phys., 62, 083305.
3. Lizarte, F. (2022) *Lower bounds for the logarithmic energy on $\mathbb{S}^2$ and for the Green energy on $\mathbb{S}^n$.* Work in progress.

Monday, July 18, 2022, 16:30 – 17:00, Lecture Hall 5

Reversible random number generators and adjoint Monte Carlo simulation for tokamak divertor design

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Special session: Developments in and Applications of MCQMC Software p.55

Nuclear fusion is an exciting potential source of clean, reliable energy for the future. However, significant challenges still remain in developing a reactor capable of supplying the power grid. One such challenge is designing the divertor, a component that removes waste particles from the reactor. The divertor comes into contact with a dense plasma, modeled as a fluid, as well as lower density neutral particles, modeled as a kinetic process.

Research codes for divertor design, such as B2-EIRENE [1], simulate the coupled plasma-neutral model through a combination of finite volume and Monte Carlo particle methods. The design is iteratively refined in an adjoint based optimization routine, i.e., gradients are computed by simulating the adjoint model with a similar discretization. The current Monte Carlo simulations are unfortunately too expensive for feasible in silico divertor design.

At KU Leuven we have developed a variety of techniques for accelerating the Monte Carlo component of these codes. We have developed a new class of asymptotic-preserving Multilevel Monte Carlo schemes [2,3] for accelerating both the forward and adjoint simulations. We have also developed a discrete adjoint approach, based on reversible random number generators. This approach simulates the same stochastic paths for the forward and adjoint Monte Carlo simulation, with the goal of reducing the number of iterations required in the optimization routine. In this talk, I will introduce these techniques, as well as our current work on challenges remaining on the path towards valorization in the B2-EIRENE code.

[1] D. Reiter, M. Baelmans, and P. Börner, *The EIRENE and B2-EIRENE Codes*, Fusion Science and Technology, 47(2), pp. 172–186, Feb. 2005

[2] E. Løvbak, G. Samaey, and S. Vandewalle, *A multilevel Monte Carlo method for asymptotic-preserving particle schemes in the diffusive limit*, Numerische Mathematik, 148(1), pp. 141186, May 2021

[3] E. Løvbak, B. Mortier, G. Samaey, and S. Vandewalle, *Multilevel Monte Carlo with Improved Correlation for Kinetic Equations in the Diffusive Scaling*, Computational Science ICCS 2020, Springer Lecture Notes in Computer Science 12142, pp. 374388, Jun. 2020

Thursday, July 21, 2022, 12:00 – 12:30, Lecture Hall 6

Rate-optimality of an adaptive quasi-Monte Carlo finite element method

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Special session: Quasi-Monte Carlo Methods of High Order and Beyond p.68

We study the Adaptive Finite Element Method for the solution of Partial Differential Equations (PDEs) governed by random coefficients, where the randomness is modeled by countably many parameters. In this talk, we show that extrapolated polynomial lattice rules allow to recover moments of the solution of a PDE, within a given error tolerance. Based on [1], we compare two approaches for adaptivity, which are non-intrusive, easily parallelizable and break the curse of dimensionality, if suitable parametric regularity assumptions are verified. Moreover, we show novel results achieving rate-optimal convergence of the finite element error, under assumptions comparable to the deterministic setting, also for certain non-linear PDEs.

[1] M. Longo. (in press). Adaptive Quasi-Monte Carlo Finite Element Methods for parametric elliptic PDEs. *J. Sci. Comput.*

Wednesday, July 20, 2022, 14:30 – 15:00, Lecture Hall 5

A multilevel stochastic approximation algorithm for unbiased value-at-risk and expected shortfall estimation

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We propose a multilevel stochastic approximation scheme [1] for the computation of the value-at-risk and the expected shortfall of a given financial loss. The financial loss can only be computed via simulations that are conditional to the realization of future risk factors. Thus, the problem at hand of estimating its value-at-risk and expected shortfall is nested in nature and can in addition be viewed as an instance of stochastic approximation problems *with a bias* as per [2]. In this framework, for a prescribed precision ε, the optimal complexity of the standard stochastic approximation algorithm is of order ε^{-3}. Thanks to the multilevel approach, we prove that the optimal complexity of our multilevel stochastic approximation algorithm is of order $\varepsilon^{-2-\delta}$, where $\delta < 1$ is a small number that depends on the integrability level of the loss. We provide some numerical results to validate our analysis.

1. Noufel Frikha. *Multi-level stochastic approximation algorithms.* Annals of Applied Probability 26.2 (2016), pp. 933985.
2. David Barrera, Stéphane Crépey, Babacar Diallo, Gersende Fort, Emmanuel Gobet and Uladzislau Stazhynski. *Stochastic Approximation Schemes for Economic Capital and Risk Margin Computations.* ESAIM: Proceedings and Surveys (2019).

Tuesday, July 19, 2022, 17:00 – 17:30, Lecture Hall 4

Multilevel delayed acceptance: ergodic MCMC for model hierarchies

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Special session: Recent Advances in MCMC Sampling Techniques p.70

We present a novel MCMC algorithm, titled Multilevel Delayed Acceptance (MLDA). The algorithm is capable of sampling from the exact target distribution using a hierarchy of distributions of increasing complexity and computational cost and can be considered as an amalgam of two existing methods, namely the Delayed Acceptance (DA) MCMC of Christen and Fox [1] and the Multilevel MCMC (MLMCMC) of Dodwell *et al.* [2].

The original DA algorithm was designed to use a single coarse distribution to filter MCMC proposals before computing the fine density. We extend this approach in two ways. *Vertically*, by allowing any number of coarse distributions to underpin the target and *horizontally*, by allowing the coarse level samplers to generate extended subchains of either fixed or random lengths. The resulting algorithm is in detailed balance with the exact target distribution. We show that MLDA can be exploited for variance reduction, similarly to MLMCMC, and construct a multilevel error model that adaptively aligns the coarse distributions to the target with little additional computational cost.

[1] Christen J. A. and Fox C. (2005), Markov chain Monte Carlo Using an Approximation. *J. Comput. Graph. Stat.*

[2] Dodwell T. J., Ketelsen C., Scheichl R., and Teckentrup A. L. (2015), A Hierarchical Multi-level Markov Chain Monte Carlo Algorithm with Applications to Uncertainty Quantification in Subsurface Flow. *SIAM/ASA J. Uncertain. Quantif.*

Monday, July 18, 2022, 15:30 – 16:00, Lecture Hall 1

High-dimension simulating hyperplane-truncated multivariate normal distributions

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Generating multivariate normal distributions is widely used in many fields (such as science and engineering). In this paper, simulating high-dimensional multivariate normal distributions truncated on the intersection of a set of hyperplanes is investigated. The proposed methodology is based on combining Karhunen-Loève expansions (KLE) and Matheron's update rules (MUR). The KLE requires the computation of the decomposition of the covariance matrix of the random variables. This step becomes expensive when the data dimension is high. To deal with this issue, the domain is split in smallest sub-domains where the eigen decomposition can be computed. In the first step, the KLE coefficients are conditioned in order to guarantee the correlation structure on the entire domain. In the second one, the assembled vectors are mapped on the intersection of a set of hyperplanes using the MUR. This technique can also be parallelized and then reduces the computational complexity.

Monday, July 18, 2022, 17:30 – 18:00, Lecture Hall 5

Hybrid deterministic/MC methods in SOLPS-ITER

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Special session: Developments in and Applications of MCQMC Software p.55

One of todays biggest challenges is to meet the growing worldwide demand of energy in a sustainable way. One of the most promising solutions is nuclear fusion energy. The realization of a profitable fusion reactor, unfortunately, comes with many technical complications. To avoid the cost of building many prototypes, computer simulations are used during the optimization phase of the reactor design.

Neutral particles play an important role in shielding the reactor walls from the hot plasma in which the fusion reactions take place. The zone where neutral particles interact with the incoming plasma and the reactor walls is called the plasma edge. The neutral particles can be described by a kinetic equation, which is difficult to solve due to the high dimensionality of the phase space and the high collisionality between the neutral particles and the plasma background, especially in the working regimes anticipated for future reactors.

SOLPS-ITER [1] is one of the few codes that is used worldwide for modeling the plasma edge. The code uses a Monte Carlo solver, called EIRENE [2], to treat the neutral particles. In the high collisional regimes a pure Monte Carlo solver becomes very expensive. To alleviate the computational cost, hybrid deterministic/MC methods that exploit the high-collisionality of the system are being introduced in EIRENE [3]. This is a challenging task as the solver was initially intended to be a pure Monte Carlo code. In this talk we will shed light on what EIRENE is, on the different deterministic/MC methods that are being implemented in EIRENE, and on how the code has to be changed to perform well with these hybrid methods, with special focus on one type of hybrid deterministic/MC method: the micro-macro hybrid approach [4].

[1] S. Wiesen et al., The new SOLPS-ITER code package, Journal of Nuclear Materials, 463, p. 480, 2015.

[2] D. Reiter, M. Baelmans and P. Börner, The EIRENE and B2-EIRENE codes, Fusion Science and Technology, 47 (2), p. 172, 2005.

[3] D.V. Borodin et al., Fluid, kinetic and hybrid approaches for neutral and trace ion edge transport modelling in fusion devices, accepted by Nuclear Fusion.

[4] N. Horsten, G. Samaey and M. Baelmans, A hybrid fluid-kinetic model for hydrogenic atoms in the plasma edge of tokamaks based on a micro-macro decomposition of the kinetic equation, Journal of Computational Physics, 409, ARTN 109308, 2020.

Monday, July 18, 2022, 11:00 – 11:30, Lecture Hall 3

QMC designs and random point configurations

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Special session: Quantifying Notions of Equidistribution on the Sphere p.66

Sequences of QMC designs, introduced in [1], provide optimal order of equal weight integration for Sobolev spaces. In this talk I will discuss the behaviour of different random configurations on the sphere as QMC designs.

[1] J. S. Brauchart, E. B. Saff, I. H. Sloan, and R. S. Womersley. QMC designs: optimal order quasi Monte Carlo integration schemes on the sphere. Math. Comput., 83(290):28212851, 2014.

Monday, July 18, 2022, 11:30 – 12:00, Lecture Hall 3

The spherical cap discrepancy of HEALPix points

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Special session: Quantifying Notions of Equidistribution on the Sphere p.66

We shall consider questions regarding the spherical cap discrepancy of deterministic point sets on the unit 2-sphere. In particular, we study the point set given by centers of pixels in the HEALPix tessellation (short for Hierarchical, Equal Area and iso-Latitude Pixelation) and show that for such a point set with N points, the spherical cap discrepancy is lower and upper bounded by order $N^{-1/2}$. This adds to the known collection of explicitly constructed sets whose discrepancy converges with order $N^{-1/2}$, matching the asymptotic order for i.i.d. random point sets. The proof of the upper bound (with explicit constant) is based on a classical approach akin to the Gauss circle problem. We also briefly discuss a jittered sampling technique that works in the HEALPix framework and yields the best-known bound $N^{-3/4}\log N$ for randomly generated point sets.

Friday, July 22, 2022, 10:00 – 10:30, Lecture Hall 6

AdaSmooth: a fast and stable SMC algorithm for online additive smoothing

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This talk will deal with a novel sequential Monte Carlo (SMC) approach to online smoothing of additive functionals in a very general class of path-space models. Hitherto, the solutions proposed in the literature suffer from either long-term numerical instability due to particle-path degeneracy or, in the case that degeneracy is remedied by particle approximation of the so-called backward kernel, high computational demands. I will present a new, function-specific additive smoothing algorithm, AdaSmooth, which is computationally fast, numerically stable and easy to implement. In order to balance optimally computational speed against numerical stability, AdaSmooth combines a (fast) naive particle smoother, propagating recursively a sample of particles and associated smoothing statistics, with an adaptive backward-sampling-based updating rule which allows the number of (costly) backward samples to be kept at a minimum. Rigorous theoretical results guaranteeing the consistency, asymptotic normality and long-term stability of the algorithm will be presented, as well as numerical results demonstrating empirically the clear superiority of AdaSmooth to existing algorithms.

- Mastrototaro, A., Olsson, J., & Alenlöv, J. (2021). Fast and numerically stable particle-based online additive smoothing: the AdaSmooth algorithm. arXiv preprint arXiv:2108.00432.

Tuesday, July 19, 2022, 17:00 – 17:30, Lecture Hall 3

Optimality of harmonic ensembles on two-point homogeneous spaces

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Special session: Energy-Minimizing Point Configurations and Measures II p.59

In many areas of mathematics, one is interested in finding point sets on manifolds that are well-distributed, in some sense. Often, finding explicit, computable examples of well-distributed point configurations can be difficult, so one may instead samples random point configurations. Taking i.i.d. uniformly distributed points proves to be too coarse of a method, as the sampled points may clump together. This issue can be avoided by creating repulsion between our random points if we generate them via determinantal point processes.

In this talk, we shall discuss random point sets on the sphere and projective spaces generated by harmonic ensembles, determinantal point processes induced by a projection kernel built from the harmonics on those spaces. On average, the resulting sampled point sets are uniformly distributed, and in fact optimal in terms of certain energies, discrepancies, and Wasserstein distance from the uniform measure.

Thursday, July 21, 2022, 17:00 – 17:30, Lecture Hall 4

Subordinated random fields and elliptic PDEs

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Special session: Multilevel and Higher-Order Approximations for Stochastic Processes, Random Fields and PDEs p.63

We present a subordination approach to generate Lvy-type discontinuous random fields on a higher dimensional spatial parameter domain. Theoretical results on the pointwise distribution, the covariance structure and the numerical approximation of these random fields are discussed. Further, we consider elliptic partial differential equations (PDEs) where the constructed fields appear in the diffusion coefficient of the equation and present numerical examples for the approximation of the solution to the corresponding random PDE using finite element methods.

Monday, July 18, 2022, 16:30 – 17:00, Lecture Hall 1

Sharp L^1-approximation of the log-Heston SDE by Euler-type methods

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Special session: Stochastic Computation and Complexity: Quadrature for SDEs and SPDEs, Stochastic Optimization, Neural Networks p.79

We study the L^1-approximation of the log-Heston SDE

$$\begin{aligned} dX_t &= \left(\mu - \frac{1}{2}V_t\right)dt + \sqrt{V_t}\left(\rho dW_t + \sqrt{1-\rho^2}dB_t\right), \\ dV_t &= \kappa(\theta - V_t)dt + \sigma\sqrt{V_t}dW_t, \end{aligned} \qquad t \in [0,T],$$

at discrete time points by equidistant explicit Euler-type methods. We establish the convergence order $1/2 - \varepsilon$ for $\varepsilon > 0$ arbitrarily small, if the Feller index $\frac{2\kappa\theta}{\sigma^2}$ of the underlying CIR process is larger than 1. Moreover, we discuss the case of a Feller index smaller than 1 and illustrate our findings by several numerical examples. Finally, we give an outlook on the generalization of our results.

Thursday, July 21, 2022, 16:30 – 17:00, Lecture Hall 3

Constructing lattice-based algorithms for multivariate function approximation with a composite number of points

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Special session: Approximation from Random Data p.54

Rank-1 lattice rules, a main family of QMC rules, are characterised by generating vectors, and the component-by-component (CBC) construction is an efficient way to construct the generating vector. In this talk, we introduce some new results in approximating multivariate one-periodic functions using function values at rank-1 lattice points. The number of points is not limited to a prime number as in currently available literature, but can take any composite value. One benefit of the generalisation to the general number of points used in approximation is that allow embedded lattice sequences in applications. The new results cannot be trivially generalised from existing results for prime number and a new proof technique is required. With some modifications, the search criterion in the CBC construction under L_2 norm can also be applied to L_∞ norm, which allows fast CBC implementations.

Tuesday, July 19, 2022, 17:00 – 17:30, Lecture Hall 5

Importance sampling methods for McKean-Vlasov type stochastic differential equations

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Special session: Variance Reduction Techniques for Rare Events p.80

We are interested in Monte Carlo methods for estimating probabilities of rare events associated with solutions to the McKean-Vlasov stochastic differential equation (MV-SDE), whose drift and diffusion coefficients depend on the law of the solution itself. The MV-SDE is approximated using the stochastic N-particle interacting system, which is a set of N coupled stochastic differential equations. Importance sampling is used to reduce high variance in Monte Carlo estimators of rare event probabilities. Optimal change of measure is methodically derived from variance minimization, yielding an N-dimensional partial differential control equation which is cumbersome to solve. This problem is circumvented by using the decoupling approach, introduced in [1], resulting in a lower dimensional control PDE. The decoupling approach necessitates the use of a double loop Monte Carlo estimator. In this context, we formulate an adaptive double loop Monte Carlo method for estimating rare event probabilities. Significant variance reduction is observed and the computational runtime for estimating rare event probabilities up to a given relative tolerance, TOL, is reduced by multiple orders, when compared to standard Monte Carlo estimators. We also formulate a novel multilevel double loop Monte Carlo (MLDLMC) method combined with importance sampling, to estimate rare events in the MV-SDE context. This reduces the order of optimal work complexity from $\mathrm{O}(TOL^{-4})$ to $\mathrm{O}(TOL^{-3})$. Our numerical experiments are carried out on the Kuramoto model from statistical physics, which models a system of coupled oscillators.

[1] Greig Smith, Goncalo dos Reis, Peter Tankov: *Importance Sampling for McKean-Vlasov SDEs.* arXiv preprint arXiv:1803.09320, 2018

Wednesday, July 20, 2022, 11:30 – 12:00, Lecture Hall 5

Benchmark of active learning methods for structural reliability analysis

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Special session: Approximate Models for Rare Event Simulation and Uncertainty Quantification p.53

Structural reliability analysis aims at assessing the safety of structures which often operate under uncertain conditions. While simulation methods have been traditionally used to accurately estimate the failure probability of the structure, they are computationally inefficient. Surrogate-based methods have been introduced as an alternative in the past decade. They consist in building a cheaper-to-evaluate proxy of the original limit-state function which is then used within a reliability estimation algorithm. Active learning pushes this concept further by constraining the surrogate limit-state function to be accurate only in some regions of interest and hence reducing the computational cost. A learning function is generally used to find such regions of interest and enrich the design of experiments (used to build the surrogate) adaptively.

In this contribution, we first carry out a survey of recent active learning reliability methods and identify an underlying and recurring scheme. We specifically show that most of the proposed methods can fit under a consistent framework, which can be defined using four ingredients: i. a surrogate model, ii. a reliability estimation algorithm, iii. a learning function and iv. a stopping criterion. By combining non-intrusively methods selected within each of these ingredients, most of the existing active learning methods can be reconstructed.

On this basis, we constructed 39 active learning strategies and performed an extensive benchmark considering a set of 20 selected reliability problems. This lead to a total of circa 12,000 problems solved. The results were analysed to identify patterns in the performance and generalization capability of different methods. Then they were synthetized into a set of recommendations for practitioners. Finally, this benchmark has allowed us to highlight the importance of surrogate models, which should be used to fully harness the potential of sophisticated reliability estimation algorithms.

References:

Moustapha, M., S. Marelli and B. Sudret (2022). Active learning for structural reliability: Survey, general framework and benchmark. Structural Safety, 96, pp. 102174.

Tuesday, July 19, 2022, 18:00 – 18:30, Lecture Hall 5

Achieving efficiency in black-box simulation of distribution tails with self-structuring importance samplers

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Special session: Variance Reduction Techniques for Rare Events p.80

Motivated by the increasing adoption of models which utilize contextual information in risk management and decision-making, this paper presents a novel Importance Sampling (IS) scheme for measuring distribution tails of objectives modeled with enabling tools such as feature-based decision rules, mixed integer linear programs, deep neural networks, etc. Conventional efficient IS approaches suffer from feasibility and scalability concerns due to the need to intricately tailor the sampler to the underlying probability distribution and the objective. This challenge is overcome in the proposed black-box scheme by automating the selection of an effective IS distribution with a transformation that implicitly learns and replicates the concentration properties observed in less rare samples. This novel approach is guided by a large deviations principle that brings out the phenomenon of self-similarity of optimal IS distributions. The proposed sampler is the first to attain asymptotically optimal variance reduction across a spectrum of multivariate distributions despite being oblivious to the underlying structure. The large deviations principle additionally results in new distribution tail asymptotics capable of yielding operational insights. The applicability is illustrated by considering contextual routing and portfolio credit risk models informed by neural networks as examples.

Wednesday, July 20, 2022, 11:00 – 11:30, Lecture Hall 4

Exact simulation of multidimensional reflected Brownian motion

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Special session: Recent Advances in Unbiased Estimation Techniques p.72

We present an exact simulation method for multidimensional reflected Brownian motion (RBM). Exact simulation in this setting is challenging because of the presence of correlated local-time-like terms in the definition of RBM. We apply recently developed so-called ε-strong simulation techniques (also known as Tolerance-Enforced Simulation) which allow us to provide a piece-wise linear approximation to RBM with ε (deterministic) error in uniform norm. A novel conditional acceptance / rejection step is then used to eliminate the error. In particular, we condition on a suitably designed information structure so that a feasible proposal distribution can be applied. If time permits, we present additional extensions.

Wednesday, July 20, 2022, 10:30 – 11:00, Lecture Hall 1

Optimal approximation of stochastic volatility models at a single point

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Special session: Stochastic Computation and Complexity: Approximation of SDEs with Non-Standard Coefficients p.77

We study the strong approximation of the stochastic volatility model

$$\begin{aligned} dX_t &= \left(r - \tfrac{1}{2} f^2\left(V_t\right)\right)dt + f\left(V_t\right)\left(\rho dW_t + \sqrt{1-\rho^2} dB_t\right), \\ dV_t &= b\left(V_t\right)dt + \sigma\left(V_t\right)dW_t, \end{aligned} \qquad t \in [0,T], \tag{5.3}$$

where $V = (V_t)_{t\in[0,T]}$ takes values in an open set $D \subseteq \mathbb{R}$, $f, b, \sigma : D \to \mathbb{R}$ are appropriate functions, $\rho \in [-1,1]$, $r \in \mathbb{R}$ and $W = (W_t)_{t\in[0,T]}$, $B = (B_t)_{t\in[0,T]}$ are independent Brownian motions. The initial values of SDE (5.3) are assumed to be deterministic, i.e. $X_0 = x_0 \in \mathbb{R}$, $V_0 = v_0 \in D$.

We analyze the minimal L^2-error for the approximation of X_T that can be obtained by arbitrary methods that use N evaluations of each Brownian motion, that is

$$e(N) = \inf_{(s_i,t_i)_{i=1,\dots,N}\in\Pi(N)} \inf_{u\in\mathcal{U}(N)} \left[\mathbb{E}\left|u(W_{s_1}, W_{s_2}, \dots, W_{s_N}, B_{t_1}, B_{t_2}, \dots, B_{t_N}) - X_T\right|^2\right]^{1/2},$$

where $\mathcal{U}(N)$ is the set of measurable functions $u : \mathbb{R}^{2N} \to \mathbb{R}$ and

$$\Pi(N) = \left\{(s_i,t_i)_{i=1,\dots,N} : \ (s_i,t_i) \in [0,T]^2, i = 1,\dots,N,\ s_N = t_N = T\right\}.$$

Under mild assumptions on SDE (5.3) we show that

$$\liminf_{N\to\infty} \sqrt{N}\, e(N) \geq \sqrt{\frac{1-\rho^2}{6}} \int_0^T \left[\mathbb{E}(f'\sigma)^2(V_t)\right]^{1/2} dt. \tag{5.4}$$

We establish also under suitable assumptions the matching upper bound (up to the factor $\sqrt{3/2} \approx 1.2247\dots$)

$$\limsup_{N\to\infty} \sqrt{N}\, e(N) \leq \sqrt{\frac{1-\rho^2}{4}} \int_0^T \left[\mathbb{E}(f'\sigma)^2(V_t)\right]^{1/2} dt. \tag{5.5}$$

Since the coefficients of SDE (1) are in particular not required to be globally Lipschitz continuous, these results extend the classical results of Clark and Cameron (1980) and Müller-Gronbach (2002).

The prototype example for SDE (5.3) is the generalized Heston model. Here (5.4) and (5.5) hold for the CEV process as volatility process V or (under additional assumptions on the Feller index) for the CIR process, respectively, as volatility process.

Tuesday, July 19, 2022, 10:30 – 11:00, Lecture Hall 5

An adaptive algorithm for integration on $\mathbb{R}^d$ using lattice rules

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Special session: Algorithmic Advancements in MCQMC Software p.51

In a recent result [1] we developed and analysed an algorithm that uses scaled lattice rules to approximate integrals $\int_{\mathbb{R}^d} f(\boldsymbol{x}) \, \mathrm{d}\boldsymbol{x}$. The convergence rate depends on the non-periodicity of the integrand function towards increasing boxes. Depending on the decay of the function and its partial mixed derivatives we can achieve a convergence of $O(n^{-\alpha+\epsilon})$, for $\epsilon > 0$ where $\alpha \in \mathbb{N}$ is the dominating mixed smoothness of f, by using a lattice sequence. For each number of points n we calculate the appropriate box $[-a(n), a(n)]^d$ with $a(n)$ governed by the decay properties of the integrand function.

In the analysis we balance three contributions to the error: the truncation error, the projection error and the lattice rule error of the projection. In the practical algorithm we need to balance two terms: the truncation error and the lattice rule error of the original non-periodic function. We introduce an adaptive algorithm which estimates these errors and then balances them.

[1] D. Nuyens, Y. Suzuki. Scaled lattice rules for integration on $\mathbb{R}^d$ achieving higher-order convergence with error analysis in terms of orthogonal projections onto periodic spaces. https://arxiv.org/abs/2108.12639, 2021.

Wednesday, July 20, 2022, 14:00 – 14:30, Lecture Hall 6

Construction methods for rank-1 lattice rules and polynomial lattice rules

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Coauthor(s): Adrian Ebert, Peter Kritzer, Dirk Nuyens, Tetiana Stepaniuk

We develop efficient algorithms for constructing point sets of high-quality quasi-Monte Carlo (QMC) methods which can be used for approximating high-dimensional integrals of multivariate functions. In particular, we study the construction of rank-1 lattice rules and polynomial lattice rules, where they are both specified by a generating vector for numerical integration in weighted function spaces such as Korobov and Walsh spaces. These construction schemes generate QMC point sets that achieve almost optimal error convergence rates in the respective function spaces. We show that the obtained error estimates become independent of the dimension under certain conditions on the weights, which are incorporated in the definitions of the considered function spaces. Consequently, the integration problem becomes tractable. Furthermore, we derive fast implementations of the construction algorithms and confirm our theoretical findings with numerical results and experiments.

[1] A. Ebert, P. Kritzer, O. Osisiogu, T. Stepaniuk. Construction of good polynomial lattice rules in weighted Walsh spaces by an alternative component-by-component construction. Mathematics and Computers in Simulation, 192(2022), pp. 399-419.

[2] A. Ebert, P. Kritzer, O. Osisiogu, T. Stepaniuk. Component-by-component digit-by-digit construction of good polynomial lattice rules in weighted Walsh Spaces. Constructive Approximation, (2021), pp. 1-45.

[3] A. Ebert, P. Kritzer, D. Nuyens, O. Osisiogu. Digit-by-digit and component-by-component construction of lattice rules for periodic functions with unknown smoothness. Journal of Complexity, 66(2021), 101555.

Wednesday, July 20, 2022, 14:00 – 14:30, Lecture Hall 4

NuZZ: numerical Zig-Zag for general models

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Markov chain Monte Carlo (MCMC) is a key algorithm in computational statistics, and as datasets grow larger and models grow more complex, many popular MCMC algorithms become too computationally expensive to be practical. Recent progress has been made on this problem through development of MCMC algorithms based on Piecewise Deterministic Markov Processes (PDMPs), irreversible processes that can be engineered to converge at a rate which is independent of the size of data. While there has understandably been a surge of theoretical studies following these results, PDMPs have so far only been implemented for models where certain gradients can be bounded, which is not possible in many statistical contexts. Focusing on the Zig-Zag process, we present the Numerical Zig-Zag (NuZZ) algorithm, which is applicable to general statistical models without the need for bounds on the gradient of the log posterior. This allows us to perform numerical experiments on: (i) how the Zig-Zag dynamics behaves on some test problems with common challenging features; and (ii) how the error between the target and sampled distributions evolves as a function of computational effort for different MCMC algorithms including NuZZ. Moreover, due to the specifics of the NuZZ algorithms, we are able to give an explicit bound on the Wasserstein distance between the exact posterior and its numerically perturbed counterpart in terms of the user-specified numerical tolerances of NuZZ.

Thursday, July 21, 2022, 16:30 – 17:00, Lecture Hall 6

Super-polynomial accuracy of median-of-means

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Special session: Quasi-Monte Carlo Methods of High Order and Beyond p.68

Digital net is an important class of Quasi-Monte Carlo methods used for numerical integration. In the talk, I am going to show digital net randomized by linear scrambling and digital shift exhibits surprising concentration behavior. Taking the median of several digital net averages can exclude outliers and boost the convergence rate from cubic to super-polynomial when the integrand is smooth. The proof is an interesting application of the Hardy-Ramanujan asymptotic formula for partition of integers.

Wednesday, July 20, 2022, 14:00 – 14:30, Lecture Hall 1

Bounds on Wasserstein distances using independent samples

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Given independent samples from two distributions, the Wasserstein distance between the samples provides a natural conservative plug-in estimator of the distance between the distributions. When these distributions are similar, the usefulness of this estimator is severely limited by its bias, which does not decay to zero with the true Wasserstein distance. We propose a linear combination of plug-in estimators for the squared 2-Wasserstein distance that reduces the bias and decays to zero with the true distance. The new estimator remains conservative provided one distribution is appropriately overdispersed with respect the other, and is unbiased when the distributions are equal. We apply it to approximately bound from above the 2-Wasserstein distance between the target and current distribution in Markov chain Monte Carlo, running multiple identically distributed chains which start, and remain, overdispersed with respect to the target. When the chains have converged, the bound asymptotes at zero in expectation. Simulations show our bound consistently outperforming the current state-of-the-art 2-Wasserstein bound for MCMC algorithms, obtaining mixing time bounds up to an order of magnitude tighter.

Wednesday, July 20, 2022, 14:30 – 15:00, Lecture Hall 3

Extremal distributions of discrepancy functions

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The irregularities of a distribution of N points in the unit interval are often measured with various notions of discrepancy. The discrepancy function can be defined with respect to intervals of the form $[0, t) \subset [0, 1)$ or arbitrary subintervals of the unit interval.In the former case, it is a well known fact in discrepancy theory that the N-element point set in the unit interval with the lowest L_2 or L_∞ norm of the discrepancy function is the centered regular grid

$$\Gamma_N := \left\{ \frac{2n+1}{2N} : n = 0, 1, \ldots, N-1 \right\}.$$

We show a stronger result on the distribution of discrepancy functions of point sets in $[0, 1]$, which basically says that the distribution of the discrepancy function of Γ_N is in some sense minimal among all N-element point sets. As a consequence, we can extend the above result to rearrangement-invariant norms, including L_p, Orlicz and Lorentz norms. We study the same problem also for the discrepancy notions with respect to arbitrary subintervals. In this case, we will observe that we have to deal with integrals of convolutions of functions. To this end, we present a general upper bound on such expressions, which might be of independent interest as well.

Thursday, July 21, 2022, 11:00 – 11:30, Lecture Hall 4

Theoretical insights on a class of control based particle filters and their approximations

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Special session: Advanced Particle Methods for Bayesian Inference p.50

In particle based filtering, ensemble Kalman type methods have in large part been the method of choice for high dimensional non-linear applications due to their desirable stability properties. This is despite the fact that they are known to be sub-optimal as they are not consistent with Bayes theorem even as the ensemble size goes to infinity. Over the last few decades, a range of so-called particle flow or control type filters have been developed which at least theoretically show strong potential over importance sampling based techniques for providing consistent estimates in high dimensional nonlinear applications.

We develop a unifying framework through which to derive and understand the links between these filters, with the aim of elucidating how alternative formulations with desirable computational properties could be designed. We show how different assumptions on the form of the control or "gain function" lead to different filters proposed in the literature. Recent work relating to accuracy, mean field limits and well-posedness of a diffusion map based approximation and its connections to other particle based methods will also be discussed.

Monday, July 18, 2022, 12:00 – 12:30, Lecture Hall 5

Generator matrices by solving integer linear programs

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Special session: Developments in and Applications of MCQMC Software p.55

In quasi Monte-Carlo methods, generating high-dimensional low discrepancy sequences by generator matrices is a popular and efficient approach. The low discrepancy is often enforced by the (t, m, s)-net property. Often, numerical problems have some intrinsic structure that benefits from a specific profile of discrepancy imposed on subsets of dimensions. Finding generator matrices that match such a profile is a historically hard problem. Many low discrepancy sequences, such as Sobol, Halton, and others, use specific matrix construction rules to achieve provably strong properties. However, these construction rules highly constrain which sort of matrices can be constructed and thus hinder efforts to match a targeted profile. The work by Joe and Kuo on optimizing the uniformity of all pairs of dimensions shows that these matrices cannot reach a satisfying 2D uniformity.Recently methods for optimizing general matrices have been devised, however they often rely on random generation and filtering of generator matrices. This approach fails when the constraints are sufficiently restrictive so that only few matrices among the search space can satisfy them. We devise a greedy algorithm allowing us to translate desirable net properties into linear constraints on the generator matrix entries. We then use these constraints in an integer linear program solver in order to directly construct matrices satisfying a desired set of net properties. We show that our method finds matrices in difficult settings, thus offering low discrepancy sequences beyond the limitations of classic matrix constructions. Some sets of constraints are provably infeasible in lower prime basis such as 2. Our method works in higher prime bases, too, offering another degree of freedom to satisfy a specific set of projective net properties.

Tuesday, July 19, 2022, 15:30 – 16:00, Lecture Hall 6

Strong invariance principles for ergodic Markov processes

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Strong invariance principles describe the error term of a Brownian approximation of the partial sums of a stochastic process. While these strong approximation results have many applications, the results for continuous-time settings have been limited. In this paper, we obtain strong invariance principles for a broad class of ergodic Markov processes. The main results rely on ergodicity requirements and an application of Nummelin splitting for continuous-time processes. Strong invariance principles provide a unified framework for analysing commonly used estimators of the asymptotic variance in settings with a dependence structure. We demonstrate how this can be used to analyse the batch means method for simulation output of Piecewise Deterministic Monte Carlo samplers.

Wednesday, July 20, 2022, 14:30 – 15:00, Lecture Hall 6

Adaptive methods for numerical approximation: an asymptotic analysis

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The crude Monte Carlo algorithm approximates the integral

$$S(f) = \int_a^b f(x)\,\mathrm{d}x$$

with expected error (deviation) $\sigma(f)N^{-1/2}$, where $\sigma(f)^2 = S(f^2) - (Sf)^2$ is the variance of f and N is the number of function evaluations. If $f \in C^r$ then special variance reduction techniques can lower this error to the level $N^{-(r+1/2)}$; however, the asymptotic constants crucially depend on the chosen technique. In this talk, we consider methods of the form

$$\overline{M}_N(f) = S(L_m f) + M_n(f - L_m f),$$

where L_m is the piecewise polynomial interpolation of f of degree $r-1$ using a partition of the interval $[a,b]$ into m subintervals, M_n is a Monte Carlo type algorithm using n samples of f, and N is the total number of function evaluations used. We derive asymptotic error formulas for the methods $\overline{M}_N$ that use nonadaptive as well as adaptive partitions. Although the convergence rate $N^{-(r+1/2)}$ cannot be beaten, the asymptotic constants make a huge difference, especially for functions f with dramatically changing rth derivative. For example, for $\int_0^1 (x+d)^{-1}\mathrm{d}x$ and $r = 4$ the best adaptive methods overcome the nonadaptive ones roughly 10^{12} times if $d = 10^{-4}$, and 10^{29} times if $d = 10^{-8}$. In addition, the adaptive methods are easily implementable and can be well used for automatic integration.

We believe that the obtained results can be generalized to multivariate integration.

Friday, July 22, 2022, 10:00 – 10:30, Lecture Hall 5

Maximum order complexity for some automatic and morphic sequences along polynomial values

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Special session: Pseudo-Random Number Generation p.65

Automatic sequences are not pseudo-random sequences since both their subword complexity and their expansion complexity are small, and their correlation measures of order 2 is large. These sequences are indeed highly predictable despite having a large maximum order complexity. However, recent results show that polynomial subsequences of automatic sequences, such as the Thue–Morse sequence, are better candidates for pseudo-random sequences. A natural generalization of automatic sequences are morphic sequences, given by a fixed point of a prolongeable morphism that is not necessarily uniform. In this talk, I will present my results on lowers bounds for the maximum order complexity of the Thue–Morse sequence, the Rudin–Shapiro sequence and the Zeckendorf sequence which is based on the sum of digits function in Fibonacci base. Theses are examples of automatic, respectively, morphic sequences.

1. Michael Drmota, Christian Mauduit, and Joël Rivat, *Normality along squares*, J. Eur. Math. Soc. (JEMS) **21** (2019), no. 2, 507548.
2. Damien Jamet, Pierre Popoli, and Thomas Stoll, *Maximum order complexity of the sum of digits function in zeckendorf base and polynomial subsequences*, Cryptography and Communications **13** (2021).
3. László Mérai and Arne Winterhof, *Pseudorandom sequences derived from automatic sequences*, 2021, https://arxiv.org/abs/2105.03086.
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Thursday, July 21, 2022, 12:00 – 12:30, Lecture Hall 3

Operator norms of random matrices with structured variance profile

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Special session: Approximation from Random Data p.54

Random matrices play a fundamental role in several areas of mathematics and understanding their spectral statistics has attracted considerable attention. Gaussian random matrices have played a fundamental role ever since. In this talk we present some results on the order of the expected operator norm of Gaussian random matrices with non-trivial variance profile, where the random Gaussian operator acts between finite-dimensional ℓ_p spaces. The goal is to understand the influence of the variance structure on the magnitude of expected norm and we present results which are optimal up to logarithmic factors in the dimension. The case of the spectral norm has been resolved by Latała, van Handel, and Youssef [Inventiones mathematicae 214(3) (2018)].

Tuesday, July 19, 2022, 17:00 – 17:30, Lecture Hall 1

Randomized Milstein algorithm for pointwise approximation of SDEs under inexact information

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Special session: Stochastic Computation and Complexity: High Dimensional Approximation, Integration, and PDEs p.78

We deal with pointwise approximation of solutions of scalar stochastic differential equations in the presence of informational noise about underlying drift and diffusion coefficients. We define randomized and derivative-free version of Milstein algorithm $\bar{\mathcal{A}}_n^{df-RM}$, and investigate its error. We also study lower bounds on the worst-case error of an arbitrary algorithm. It turns out that in some case the scheme $\bar{\mathcal{A}}_n^{df-RM}$ is the optimal one. Finally, in order to test the algorithm $\bar{\mathcal{A}}_n^{df-RM}$ in practice, we report performed numerical experiments.

[1] P. Morkisz, P. Przybyłowicz. *Randomized derivative-free Milstein algorithm for efficient approximation of solutions of SDEs under noisy information.* Journal of Computational and Applied Mathematics, **383** (2021), 1-22.

Thursday, July 21, 2022, 11:30 – 12:00, Lecture Hall 1

Strong and weak approximation of solutions of SDEs under noisy information about coefficients and driving Wiener process

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Special session: Stochastic Computation and Complexity: Approximation of SDEs with Non-Standard Coefficients p.77

We investigate approximation, in strong and weak sense, of solutions of the following stochastic differential equations (SDEs)

$$\begin{cases} X(t) = a(t, X(t))dt + b(t, X(t))dW(t), \ t \in [0, T], \\ X(0) = \eta, \end{cases} \tag{5.6}$$

where $T > 0$, and W is a m-dimensional Wiener process. We assume that only standard noisy information about the coefficients a, b and driving Wiener process W is available. In the case of strong approximation, we show the upper bound $O(n^{-\min\{1/2,\varrho\}} + \delta_1 + \delta_2 + \delta_3)$ on the $L^p(\Omega)$-error for the randomized Euler algorithm, where n is the discretization parameter, $\varrho \in (0, 1]$ is the Hölder exponent wrt to the time variable t for $b = b(t, x)$, and $\delta_1, \delta_2, \delta_3$ are precision parameters for a, b, W, respectively. We also show some lower bounds. Next, we construct a suitable Monte Carlo algorithm that approximates $\mathbb{E}(F(X(T)))$. In this case we also assume that we have available standard noisy information about the pay-off function F. We apply the obtained results to the problem of approximation of solutions of PDEs under noisy information about their coefficients. Results of some numerical experiments performed on GPUs are going to be reported.

Wednesday, July 20, 2022, 12:00 – 12:30, Lecture Hall 3

On the Fourier sign uncertainty principle

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Special session: What Did You Expect? Equidistribution in Number Theory p.81

There has been recent progress in studying point distributions via harmonic analysis tools. In 2003, Cohn and Elkies introduced new upper bounds for sphere packings via a Fourier optimization problem. It was solved exactly in the special dimensions 8 and 24, in a recent breakthrough by Viazovska and Cohn, Kumar, Miller, Radchenko and Viazovska. As later pointed out by Cohn and Gonalves, this is deeply related to the classical topic of Fourier uncertainty, and specifically to an uncertainty principle regarding the signs of a function and its Fourier transform.

We discuss a generalized version of the Fourier sign uncertainty principle in Euclidean space, based on joint work with Emanuel Carneiro.

Thursday, July 21, 2022, 17:30 – 18:00, Lecture Hall 4

Higher-order adaptive numerical methods for computing the exit times of stochastic processes

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Special session: Multilevel and Higher-Order Approximations for Stochastic Processes, Random Fields and PDEs p.63

The task of computing the time taken by a stochastic process to exit a domain or reach a certain value is of great interest and has applications in the fields of science and finance. In physics, one might be interested in computing the time taken by a particle in a potential well to cross over a potential barrier. In finance, an investor would be interested in knowing the time when the stock/option exceeds a certain threshold value in order to sell the stock/option and maximize profit. Computing the mean exit time of a stochastic process relates to solving a deterministic PDE, but solving the PDE is oftentimes neither feasible analytically nor tractable numerically. So we resort to Monte Carlo techniques using sample paths of the stochastic process in order to estimate the mean exit time. By sampling the trajectories of the stochastic process at discrete times, we run the risk of missing the exit in-between timesteps.

We propose an alternative method to compute the mean exit time of a stochastic process that aims at minimizing the probability of missing the exit by refining the timestep size as the stochastic process gets closer to the boundary. As a consequence, we are able to achieve higher-order convergence rates while keeping the expected computational cost low. In this talk we will explain the structure of our adaptive method and compare its performance to the state of the art by looking at some numerical examples. As our method currently is a single-level Monte Carlo method, we will also discuss the potential of our method when extended to the multilevel Monte Carlo setting.

Thursday, July 21, 2022, 10:30 – 11:00, Lecture Hall 5

State and parameter estimation from partial state observations in stochastic reaction networks

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Special session: Monte Carlo Methods and Variance Reduction Techniques for Stochastic Reaction Networks p.62

We describe new Monte Carlo methods for the accurate and efficient estimation of unobserved states and parameters of a stochastic reaction network based on exact partial state observations. We consider two scenarios, one in which the observations are made continuously in time over a window and the other in which observations are made in snapshots of time. We provide particle filter algorithms for the estimation of the conditional probability distribution of the states and parameters. We provide derivations of our methods as well as as numerical examples that illustrate the applicability of our approach.

[1] "State and parameter estimation from exact partial state observation in stochastic reaction networks" Muruhan Rathinam and Mingkai Yu, J. Chem. Phys. 154, 034103 (2021).

Wednesday, July 20, 2022, 12:00 – 12:30, Lecture Hall 1

On the performance of the Euler-Maruyama scheme for multidimensional SDEs with discontinuous drift coefficient

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Special session: Stochastic Computation and Complexity: Approximation of SDEs with Non-Standard Coefficients p.77

We study the performance of the Euler-Maruyama scheme for systems of SDEs with a piecewise Lipschitz drift coefficient and a Lipschitz diffusion coefficient. We show that an L_p-error rate of at least $1/2-$ is achieved, which generalizes a recent result from [2] for scalar SDEs and improves the known L_2-error rate of at least $1/4$ from [1] for the multi-dimensional setting.

[1] Leobacher, G. and Szölgyenyi, M. (2018), *Convergence of the Euler-Maruyama method for multidimensional SDEs with discontinuous drift and degenerate diffusion coefficient*, Numerische Mathematik **138**, 219–239.

[2] Müller-Gronbach, T. and Yaroslavtseva, L. (2020), *On the performance of the Euler-Maruyama scheme for SDEs with discontinuous drift coefficient*, Ann. Inst. H. Poincaré Probab. Statist. **56**, 1162–1178.

Tuesday, July 19, 2022, 16:00 – 16:30, Lecture Hall 4

Multi-fidelity no-U-turn sampling

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Many Markov Chain Monte Carlo (MCMC) methods often take many iterations to converge for highly correlated or high-dimensional target density functions. Methods such as Hamiltonian Monte Carlo (HMC) [1] or No-U-Turn Sampling (NUTS) [2] use the first-order derivative of the density function to tackle the aforementioned issues. However, the calculation of the derivative represents a bottleneck for computationally expensive models. We propose to first build a multi-fidelity Gaussian Process (GP)[3, 4, 5] surrogate. The building block of the multi-fidelity surrogate is a hierarchy of models of decreasing approximation error and increasing computational cost. Then the generated multi-fidelity surrogate is used to approximate the derivative. The majority of the computation is assigned to the cheap models thereby reducing the overall computational cost. The derivative from the multi-fidelity method is used to explore the target density function and generate proposals. We select or reject the proposals using the Metropolis Hasting criterion using the highest fidelity model which ensures that the proposed method is ergodic with respect to the highest fidelity density function. We apply the proposed method to some test cases and compare it with existing methods.

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Monday, July 18, 2022, 17:00 – 17:30, Lecture Hall 1

A posteriori error estimates for fully coupled McKean-Vlasov FBSDEs

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Special session: Stochastic Computation and Complexity: Quadrature for SDEs and SPDEs, Stochastic Optimization, Neural Networks p.79

McKean-Vlasov forward-backward stochastic differential equations (MV-FBSDEs) with full coupling arise naturally from large population optimization problems. Judging the quality of given numerical solutions for MV-FBSDEs, which usually require Picard iterations and approximations of nested conditional expectations, is typically difficult. This talk proposes an a posteriori error estimator to quantify the L^2-approximation error of an arbitrarily generated approximation on a time grid. We establish that the error estimator is equivalent to the global approximation error between the given numerical solution and the solution of a forward Euler discretized MV-FBSDE. A crucial and challenging step in the analysis is the proof of stability of this Euler approximation to the MV-FBSDE, which is of independent interest. We further demonstrate that, for sufficiently fine time grids, the accuracy of numerical solutions for solving the continuous MV-FBSDE can also be measured by the error estimator. In particular, the a posteriori error estimates justify the usage of the Deep BSDE Solver for solving MV-FBSDEs. Numerical experiments on an extended mean field game are presented to illustrate the theoretical results and to demonstrate the practical applicability of the error estimator.

Friday, July 22, 2022, 10:00 – 10:30, Lecture Hall 3

Convergence of a time-stepping scheme to the free boundary in the supercooled Stefan problem

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Special session: Analysis and Simulation of SDEs in Non-standard Settings p.52

The supercooled Stefan problem and its variants describe the freezing of a supercooled liquid in physics, as well as the large system limits of systemic risk models in finance and of integrate-and-fire models in neuroscience. Adopting the physics terminology, the supercooled Stefan problem is known to feature a finite-time blow-up of the freezing rate for a wide range of initial temperature distributions in the liquid. Such a blow-up can result in a discontinuity of the liquid-solid boundary. In this paper, we prove that the natural Euler time-stepping scheme applied to a probabilistic formulation of the supercooled Stefan problem converges to the liquid-solid boundary of its physical solution globally in time, in the Skorokhod M1 topology. In the course of the proof, we give an explicit bound on the rate of local convergence for the time-stepping scheme. We also run numerical tests to compare our theoretical results to the practically observed convergence behavior.

Monday, July 18, 2022, 16:00 – 16:30, Lecture Hall 6

Eliminating sharp minima from SGD with truncated heavy-tailed noise

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The empirical success of deep learning is often attributed to SGD's mysterious ability to avoid sharp local minima in the loss landscape, as sharp minima are known to lead to poor generalization. Recently, empirical evidence of heavy-tailed gradient noise was reported in many deep learning tasks, and it was shown that SGD can escape sharp local minima under the presence of such heavy-tailed gradient noise, providing a partial solution to the mystery. In this work, we analyze the metastability of a popular variant of SGD where gradients are truncated above a fixed threshold. We show that such SGD achieves a stronger notion of avoiding sharp minima: it can effectively eliminate sharp local minima entirely from its training trajectory. We show this by characterizing the dynamics of truncated SGD driven by heavy-tailed noises. First, we prove that the truncation threshold and width of the attraction field dictate the order of the first exit time from the associated local minimum. Moreover, when the loss landscape satisfies appropriate structural conditions, we prove that, as the learning rate decreases, the dynamics of heavy-tailed truncated SGD closely resemble those of a continuous-time Markov chain that never visits any sharp minima. Real data experiments on deep learning confirm our theoretical prediction that heavy-tailed SGD with gradient clipping finds a flatter local minima and achieves better generalization.

Tuesday, July 19, 2022, 11:30 – 12:00, Lecture Hall 4

Metropolis adjusted Langevin trajectories: a robust alternative to Hamiltonian Monte Carlo

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Special session: Robust Innovations in Gradient-Based MCMC p.73

Hamiltonian Monte Carlo (HMC) is a widely used sampler, known for its efficiency on high dimensional distributions. Yet HMC remains quite sensitive to the choice of integration time. Randomizing the length of Hamiltonian trajectories (RHMC) has been suggested to smooth the Auto-Correlation Functions (ACF), ensuring robustness of tuning. We present the Langevin diffusion as an alternative to control these ACFs by inducing randomness in Hamiltonian trajectories through a continuous refreshment of the velocities. We connect and compare the two processes in terms of quantitative mixing rates for the 2-Wasserstein and $\mathbb{L}_2$ distances. The Langevin diffusion is presented as a limit of Randomised Hamiltonian dynamics achieving the fastest mixing rate for strongly log-concave targets. We introduce a robust alternative to HMC built upon these dynamics, named Metropolis adjusted Langevin trajectories (MALT). Studying the scaling limit of MALT, we obtain optimal tuning guidelines similar to HMC, and recover the same scaling with respect to the dimension without additional assumptions. We illustrate numerically the efficiency of MALT compared to HMC and RHMC.

Thursday, July 21, 2022, 16:00 – 16:30, Lecture Hall 3

Equivalence of integration on Gaussian spaces and Hermite spaces

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We study integration of functions of d variables with respect to the d-fold product of the standard normal distribution, where $d \in \mathbb{N}$ or $d = \infty$. The underlying function space is a reproducing kernel Hilbert space whose kernel L_σ is the tensor product of univariate Gaussian kernels with shape parameters $\sigma_j > 0$, i.e., $L_\sigma(x, y) := \prod_{j=1}^{d} \exp(-\sigma_j^2 \cdot (x_j - y_j)^2)$. For every Gaussian kernel L_σ (with square-summable shape parameters if $d = \infty$) we determine a Hermite kernel K_σ such that the integration problem on the Gaussian space $H(L_\sigma)$ is equivalent to the same integration problem on the Hermite space $H(K_\sigma)$. More precisely, there is a one-to-one correspondence between quadrature formulas on $H(L_\sigma)$ and $H(K_\sigma)$ such that the worst case errors on the corresponding unit balls coincide. The proof is constructive, and a similar result, however with a different Hermite kernel, holds for L^2-approximation.

Monday, July 18, 2022, 17:00 – 17:30, Lecture Hall 5

Bayesian calibration for summary statistics with applications to a cluster dynamics model

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Special session: Developments in and Applications of MCQMC Software p.55

We present a Bayesian calibration strategy for problems where observed data summaries are available as measurement values with associated measurement errors, where the latter are represented by error bars. Our method finds a collection of synthetic data sets, such that statistics computed from the pushed forward posterior (i.e., the parameter values after observing the data, propagated through the deterministic model) are consistent with the reported summary statistics. In doing so, the reported measurement errors are reflected in the inferred uncertain parameters. We apply our method to a cluster dynamics model for the prediction of uranium and xenon fission gas diffusivity and oxygen non-stoichiometry in uranium dioxide nuclear fuel. To keep the approach computationally tractable, we replace the cluster dynamics model with a prebuilt polynomial surrogate mode. The observed summary statistics used in our calibration effort are taken from various sources in the literature. We discuss the performance of the algorithm, and investigate how we can introduce weights to account for the different number of measurement values in each experimental data set. We implement our approach in UQTk, a software package developed at Sandia.

Thursday, July 21, 2022, 15:30 – 16:00, Lecture Hall 6

Multilevel simulation of hard sphere mixtures

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We present a self-consistent multilevel simulation method to estimate equilibrium properties of multiscale physical systems. Inspired by multilevel Markov chain Monte Carlo methods, we use an efficient but inexact coarse-grained approximation as the starting point of a hierarchical method to simulate the exact system of interest. We apply this method to highly size-asymmetric binary mixtures of hard spheres, where the scale separation between big and small particles poses a substantial challenge to standard Monte Carlo simulation methods. The big particles of this system display interesting collective behaviour, including a de-mixing transition at large size-ratios and high small-particle densities. To investigate this system, we first develop a two-level method that enables us to simulate the system up to this transition, providing the first computational evidence of its existence and locating the associated critical point [1]. Subsequently, we discuss a generalisation of the two-level method that makes use of multiple levels of physical coarse-graining, and apply a three-level version to the binary mixture. For this example, we compare the numerical and asymptotic performance of the two- and three-level method. We show that taking an intermediate level into account can lower the variance of the method at fixed computational cost.

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Thursday, July 21, 2022, 11:30 – 12:00, Lecture Hall 4

A kernelized consensus-based optimization method

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Special session: Advanced Particle Methods for Bayesian Inference p.50

Consensus-based optimization (CBO) [1] is a derivative-free method for minimizing a function $V : \mathbb{R}^d \to \mathbb{R}$ by evolving an ensemble of particles towards its mean value with respect to the Gibbs measure $\exp(-\beta V)$ where $\beta > 0$ is an inverse heat parameter. After long time the ensemble will concentrate close to a minimizer of V. Generalizations of CBO to sampling also exist [2]. While being computationally efficient, these methods are of limited use for minimizing non-convex functions or sampling from multi-modal distributions, basically because the whole ensemble follows one common mean value. In this talk I present a novel CBO method which uses a kernelized notion of mean value. This kernelized mean is different for every particle and—for kernels $k(x, y)$ which are decreasing functions of the distance between x and y—coincides with a weighted average of close-by points. This way the proposed method allows for finding several global minima of non-convex functions and for multi-modal sampling. I will present numerical examples and first theoretical results on this novel method.

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Tuesday, July 19, 2022, 10:30 – 11:00, Lecture Hall 1

Geometric convergence of polar slice sampling

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Special session: Stochastic Computation and Complexity: High Dimensional Approximation, Integration, and PDEs p.78

Roberts and Rosenthal introduced and analyzed in [1] the polar slice sampler for approximate sampling w.r.t. a posterior target distribution on $\mathbb{R}^d$. They showed that it performs, in contrast to other sampling methods, dimension independent, at least if suitably initialized and if the posterior density satisfies some structural properties. By extending arguments of [2] we prove that it has a particularly simple, explicit and dimension-independent spectral gap for strictly increasing, convex and twice differentiable negative log density functions.

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Monday, July 18, 2022, 17:30 – 18:00, Lecture Hall 6

Quasi-Monte Carlo methods and discontinuous Galerkin

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In this talk, we design and develop Quasi-Monte Carlo (QMC) cubatures for non-conforming discontinuous Galerkin approximations of elliptic PDE problems with random coefficients. In particular, we are interested in using QMC cubatures to compute the response statistics (expectation and variance) of the discretized PDE problem and we derive rigorous QMC convergence rates for this problem.

Monday, July 18, 2022, 11:30 – 12:00, Lecture Hall 1

Recent advances of Euler-Krylovs polygonal approximations in ML and AI

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Special session: Stochastic Computation and Complexity: Quadrature for SDEs and SPDEs, Stochastic Optimization, Neural Networks p.79

The idea of using a new form of Eulers polygonal approximations, one which allows coefficients to depend directly on the step size, was highlighted in [1] and [2]. More recently, this new form of Eulers polygonal approximations has been used to create new, stochastic (adaptive) optimization algorithms with superior performance, in many cases, than other leading optimization algorithms within the context of fine tuning of artificial neural networks, see [3] and [4]. Key findings of this new methodology will be reviewed, with particular focus on the latter two references.

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Tuesday, July 19, 2022, 15:30 – 16:00, Lecture Hall 5

Robust control variates optimization for rendering

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Monte Carlo integration is a recurrent problem in computer graphics. This numerical estimation is error prone and many methods have been developed to limit it magnitude. One of them is the use of control variate to simplify the integration problem. When using a suitable control variate, it is possible to significantly reduce the complexity of the integration problem and thus the amount of error produced. On the other hand, using the bad control variate can increase the error. The major difficulty of these methods is to choose robustly these control variate. We propose an optimization-based method that ensures a variance reduction compared to a Monte Carlo estimator. This method uses the samples of a Monte Carlo estimator to build a reliable estimate of the integrated function. We then use this estimate as a control variate function. Under certain simple conditions, it is provable that this estimator has a reduced variance over to a Monte Carlo one. This method can be used as a substitute of Monte Carlo estimator in many problems. We have demonstrated its applicability to different light transport simulation problems.

Wednesday, July 20, 2022, 14:30 – 15:00, Lecture Hall 1

Ensuring unbiased sampling of HMC schemes for non separable Hamiltonian systems

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Hamiltonian Monte Carlo (or Hybrid Monte Carlo) [1] is a Markov Chain Monte Carlo method that allows to sample high dimensional probability measures. Girolami *et al.* [2] have used it to include a position-dependent diffusion coefficient, coming from the overdamped Langevin dynamics, that improves the convergence of the numerical method. It however requires simulating Hamiltonian dynamics with a non separable Hamiltonian, which is done in practice with implicit methods in order to ensure the preservation of key properties of the Hamiltonian dynamics (symplecticity and time-reversibility in particular) [3]. Unfortunately, actual implicit numerical schemes cannot be reversible, as already noted in the context of constrained stochastic differential equations [4,5]. We show here how to enforce the numerical reversibility of the method to guaranteed that the sampling is unbiased. Our numerical results demontrate that this correction is indeed relevant in practice.

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Thursday, July 21, 2022, 16:30 – 17:00, Lecture Hall 5

Modeling a life insurers balance sheet and analyzing its long-term stability

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Special session: Simulation and Monte Carlo Methods in Quantitative Finance and Insurance p.74

We devise a stochastic asset-liability management model for a life insurance company. A flexible procedure for the generation of insurers compressed contract portfolios that respects the given biometric structure is presented. The introduced balance sheet model is in line with the principles of double-entry bookkeeping as required in accounting. We prove the consistency of the balance sheet equations. We further focus on the incorporation of new business, i.e. the addition of newly concluded contracts and thus of insured in each period. Efficient simulations are retained by integrating new policies into existing cohorts according to contract-related criteria. In extensive Monte Carlo simulation studies for different scenarios regarding the business form of todays life insurers, we utilize these to analyze the long-term behavior and the stability of the components of the balance sheet for different asset-liability approaches and interest rate scenarios. Finally, we investigate the robustness of two prominent investment strategies against crashes in the capital markets, which lead to extreme liquidity shocks and thus threaten the insurers financial health. We discuss the relevance of the results based on possible simulation errors and model parameters.

Friday, July 22, 2022, 09:00 – 09:30, Lecture Hall 1

Convergence of adaptive stochastic collocation with finite elements

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Special session: Smoothing and Adaptive Methods p.75

In [1], we approximate a partial differential equation with random data using sparse grids (a collocation method) in the probability space and finite elements in the spatial domain. Both methods are adaptive: The set of collocation points used in the probability space is enlarged and the finite element meshes are refined. The adaptive refinement is steered by the reliable a-posteriori error estimator proposed in [2]. Our main result is a convergence proof of the adaptive algorithm. The analysis consists of two steps: First, we establish convergence of the semi-discrete (probability space only) scheme. Then, we extend the result to the fully discrete setting employing convergence properties of h-adaptive finite elements. To our knowledge, this is the first convergence proof of an adaptive stochastic collocation-finite elements scheme. Furthermore, we present numerical tests to validate the theoretical results and discuss the performance of the algorithm.

1. M. Feischl, and A. Scaglioni, *Convergence of adaptive stochastic collocation with finite elements*, Computers & Mathematics with Applications. 98:139–156, 2021.
2. D. Guignard, and F. Nobile, *A posteriori error estimation for the stochastic collocation finite element method*, SIAM J. Numer. Anal. 56(5):3121–3143, 2018.

Tuesday, July 19, 2022, 17:30 – 18:00, Lecture Hall 3

On the support of minimizers of causal variational principles on the sphere

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Special session: Energy-Minimizing Point Configurations and Measures II p.59

As an approach for formulating relativistic quantum field theory, causal variational principles have been proposed in [1]. In one setting, the aim of such causal variational principles is to minimize an action defined as the double integral of special non-negative functions (so-called *Lagrangians*) within the class of regular Borel probability measures on the two-sphere. We show that depending on the chosen Lagrangian, minimizers of these principles either satisfy certain properties (we call these minimizers *generically timelike*) or else have singular support (see [2]). In the latter case, it can be proven that the support of every minimizing measure is contained in a finite number of smooth curves which intersect at a finite number of points, or that the support has Hausdorff dimension at most 6/7 (see [3]). Numerical results supplement our investigations.

[1] Felix Finster, *The Continuum Limit of Causal Fermion Systems*, Fundamental Theories of Physics, vol. 186, Springer, 2016.

[2] F. Finster, D. Schiefeneder, *On the support of minimizers of causal variational principles*, Arch. Ration. Mech. Anal. 210 (2013), no. 2, 321-364.

[3] L. Bäuml, F. Finster, H. von der Mosel, and D. Schiefeneder, *Singular support of minimizers of the causal variational principle on the sphere*, Calc. Var. Partial Differential Equations 58 (2019), no. 6, 205.

Tuesday, July 19, 2022, 17:30 – 18:00, Lecture Hall 4

Convergence of unadjusted Hamiltonian Monte Carlo for mean-field models

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Special session: Recent Advances in MCMC Sampling Techniques p.70

We study unadjusted Hamiltonian Monte Carlo (uHMC) and present dimension-free convergence bounds for the uHMC algorithm applied to high-dimensional probability distributions of mean-field type. These bounds require the discretization step to be sufficiently small, but do not require strong convexity of either the unary or pairwise potential terms present in the mean-field model. To handle high dimensionality, our proof uses a particlewise coupling that is contractive in a complementary particlewise metric. Moreover, we provide quantitative discretization error bounds for uHMC. The talk is based on [1].

[1] Convergence of unadjusted Hamiltonian Monte Carlo for mean-field models, Nawaf Bou-Rabee and Katharina Schuh, ArXiv preprint arXiv:2009.08735, 2020.

Friday, July 22, 2022, 09:30 – 10:00, Lecture Hall 3

Regular conditional distributions for semimartingale SDEs

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Special session: Analysis and Simulation of SDEs in Non-Standard Settings p.52

In this talk an existence result for the regular conditional distribution a large class of semimartingale driven SDEs is presented. For this we show that the solution of these SDEs can be written as a measurable function of its driving processes into the space of all cdlg functions equipped with the Borel algebra generated by all open sets with respect to the Skorohod metric. Our result is relevant, for example, in computational stochastics: as corollary it provides a Markov property which is essential for proving convergence results of numerical methods for general semi-martingale driven SDEs.

[1] P. Przybyłowicz, V. Schwarz, M. Szölgyenyi. *Regular conditional distributions for semimartingale SDEs* (2022), preprint: https://arxiv.org/pdf/2201.06278.pdf.

Tuesday, July 19, 2022, 11:30 – 12:00, Lecture Hall 5

Connecting advanced models and advanced UQ: the MIT UQ library (MUQ) and a universal UQ/model interface

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Special session: Algorithmic Advancements in MCQMC Software p.51

Mathematical models of complex real-world phenomena result in computational challenges, necessitating advanced software and High Performance Computing systems. Uncertainty quantification (UQ) on such models is even more challenging, since uncertainties essentially increase dimensionality of the problem at hand.

Addressing those challenges, we present a Multilevel Markov Chain Monte Carlo [1] framework within the MIT Uncertainty Quantification Library (MUQ) [2]. This framework exploits model hierarchies for efficiency and allows for massive parallelism despite data dependencies in the algorithm. We show a demonstration applying it to a Bayesian inverse problem on a shallow water PDE modelling the 2011 Tohoku tsunami [3].

We further introduce UM-Bridge, a new software framework for coupling arbitrary model codes with arbitrary UQ packages, regardless of the respective software tools used. UM-Bridge makes it easy to apply advanced UQ methods on challenging models, while offering model portability through (optional) containerization as well as separation of concerns between model experts and UQ developers.

Finally, a work-in-progress set of standardized UQ benchmarks based on UM-Bridge is presented, inviting the community to get involved in their definition and implementation.

[1] Multilevel Markov Chain Monte Carlo, T. J. Dodwell, C. Ketelsen, R. Scheichl, A. L. Teckentrup, SIAM Review, https://doi.org/10.1137/19M126966X

[2] MUQ: The MIT Uncertainty Quantification Library, M. Parno, A. Davis, L. Seelinger, Journal of Open Source Software, https://doi.org/10.21105/joss.03076

[3] High Performance Uncertainty Quantification with Parallelized Multilevel Markov Chain Monte Carlo, L. Seelinger, A. Reinarz, L. Rannabauer, M. Bader, P. Bastian, R. Scheichl, The International Conference for High Performance Computing, Networking, Storage, and Analysis 2021, https://doi.org/10.1145/3458817.3476150

Monday, July 18, 2022, 15:30 – 16:00, Lecture Hall 6

Multilevel Monte Carlo with machine learned surrogate models for resource adequacy assessment

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Monte Carlo (MC) simulation is often used to evaluate the reliability of large electrical power grids. The impact of stochastic equipment outages and operating conditions is analysed with the aim to quantify risks to delivery of energy to customers. Today's grids rapidly increase in complexity, so that the evaluation of a single state can be computationally demanding. Moreover, the power system is highly reliable, and failure states that significantly affect reliability evaluation are rare. Hence, many states should be evaluated in MC simulations to obtain the desired level of accuracy, which makes the simulation computationally expensive.

Many efforts have been made to make the simulation faster. Among them, Multilevel Monte Carlo (MLMC) is one the most powerful methods that can be applied to obtain speedup computation without compromising model complexity and accuracy. High speedups can be achieved when making use of multiple models with high pair-wise correlations and large differences in evaluation speed [1]. Therefore, having good combinations of models has a significant effect on MLMC performance. However, manually constructing models with the above conditions [2] may require substantial domain knowledge. In this talk we demonstrate how machine-learned surrogate models are able to fulfil this role without resorting to careful development of approximate models. Different strategies for constructing and training surrogate models are discussed. A resource adequacy case study based on the Great Britain system with storage units is used to demonstrate the effectiveness of the proposed approach, and the sensitivity to surrogate model accuracy. The high accuracy and inference speed of machine-learned surrogates result in very large speedups, compared to using MLMC with only hand-built models.

[1] M. B. Giles, Multilevel monte carlo methods, Acta numerica, vol. 24, pp. 259328, 2015.

[2] S. Tindemans and G. Strbac, Accelerating system adequacy assessment using the multilevel monte carlo approach, Electric Power Systems Research, vol. 189, p. 106 740, 2020.

Tuesday, July 19, 2022, 12:00 – 12:30, Lecture Hall 4

The Apogee-to-Apogee Path Sampler

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Special session: Robust Innovations in Gradient-Based MCMC p.73

Amongst Markov chain Monte Carlo algorithms, Hamiltonian Monte Carlo (HMC) is often the algorithm of choice for complex, high-dimensional target distributions; however, its efficiency is notoriously sensitive to the choice of the integration-time tuning parameter. When integrating both forward and backward in time using the same leapfrog integration step as HMC, the set of *apogees*, local maxima in the potential along a path, is the same whatever point (position and momentum) along the path is chosen to initialise the integration. We present the Apogee to Apogee Path Sampler (AAPS), which utilises this invariance to create a simple yet generic methodology for constructing a path, proposing a point from it and accepting or rejecting that proposal so as to target the intended distribution. We demonstrate empirically that AAPS has a similar efficiency to HMC but is much more robust to the setting of its equivalent tuning parameter, the number of apogees that the path crosses, K.

Tuesday, July 19, 2022, 11:30 – 12:00, Lecture Hall 1

s-numbers of embeddings of weighted Wiener classes

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Special session: Stochastic Computation and Complexity: High Dimensional Approximation, Integration, and PDEs p.78

In my talk I will discuss the behaviour of some s-numbers (including approximation numbers) of three different types of embeddings of the weighted Wiener algebra $A_w(\mathbb{T}^d)$ defined on the d-dimensional torus:

- $A_w(\mathbb{T}^d) \to A(\mathbb{T}^d)$, where $A(\mathbb{T}^d)$ denotes the Wiener algebra itself;
- $A_w(\mathbb{T}^d) \to L_2(\mathbb{T}^d)$;
- $A_w(\mathbb{T}^d) \to H^1(\mathbb{T}^d)$, where w is given by

$$w(k) = w_{s,r}(k) := \begin{cases} \prod_{i=1}^d (1 + |k_i|^r)^{s/r} & \text{if} \quad 0 < r < \infty\,; \\ \prod_{i=1}^d \max(1, |k_i|)^s & \text{if} \quad r = \infty\,. \end{cases}$$

It will be the main aim of my talk to describe the behaviour of the associated s-numbers in dependence of n and the dimension d.

Tuesday, July 19, 2022, 16:30 – 17:00, Lecture Hall 1

The power of random information for recovery in ℓ_2

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Special session: Stochastic Computation and Complexity: High Dimensional Approximation, Integration, and PDEs p.78

Linear functionals can be used to recover objects in (quasi-)normed spaces with a high but finite dimension. We study the effectiveness of a random (Gaussian) choice of linear functionals compared to optimal linear functionals when the error of recovery is measured in ℓ_2. We give an overview of existing results and present new results for normed spaces whose unit balls are generalized ellipsoids, which are images of ℓ_p-balls under diagonal operators. Depending on the lengths of the semiaxes, random linear functionals may be either close to optimal or almost useless with high probability.

Tuesday, July 19, 2022, 11:00 – 11:30, Lecture Hall 5

Quasi-Monte Carlo for vector functions of integrals

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Special session: Monte Carlo and Quasi-Monte Carlo Software p.51

Quasi-Monte Carlo methods present an efficient approach for multivariate numerical integration. Algorithms exist to adaptively sample the integrand until a user defined error tolerance is satisfied with theoretical guarantees or with high probability. This work describes our extension of such methods to support adaptive sampling to satisfy error criteria for vector functions of multiple integrals. Although several functions involving multiple integrals are being evaluated, only one low discrepancy sequence is required, albeit sometimes of larger dimension than the integration domain. These enhanced algorithms are implemented in the QMCPy Python package with support for vectorized, economical integrand evaluation. Motivating examples include the approximation of sensitivity indices, coefficients for Bayesian logistic regression, and vectorized acquisition function values in Bayesian optimization.

Monday, July 18, 2022, 11:30 – 12:00, Lecture Hall 4

Monte Carlo variance reduction using Stein operators

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Special session: Developments in Markov Chain Monte Carlo p.56

This talk will focus on two new methods for estimating posterior expectations when the derivatives of the log posterior are available. The proposed methods are in a class of estimators that use Stein operators to generate control variates or control functionals. The first method [1] applies regularisation to improve the performance of popular Stein-based control variates for high-dimensional Monte Carlo integration. The second method [2], referred to as semi-exact control functionals (SECF), is based on control functionals and Sards approach to numerical integration. The use of Sards approach ensures that our control functionals are exact on all polynomials up to a fixed degree in the Bernstein-von-Mises limit. Several Bayesian inference examples will be used to illustrate the potential for reduction in mean square error.

[1] South, L. F., Oates, C. J., Mira, A., & Drovandi, C. Regularised zero-variance control variates. *arXiv preprint arXiv:1811.05073.*

[2] South, L. F., Karvonen, T., Nemeth, C., Girolami, M., & Oates, C. (2021). Semi-Exact Control Functionals From Sard's Method. *Biometrika.*

Tuesday, July 19, 2022, 16:00 – 16:30, Lecture Hall 6

Efficient computation of linear response of nonequilibrium stochastic dynamics

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Transport coefficients, such as the mobility, thermal conductivity and shear viscosity, are quantities of prime interest in statistical physics. At the macroscopic level, transport coefficients relate an external forcing of magnitude η, with $\eta \ll 1$, acting on the system to an average response expressed through some steady-state flux. In practice, steady-state averages involved in the linear response are computed as time averages over a realization of some stochastic differential equation. Variance reduction techniques are of paramount interest in this context, as the linear response is scaled by a factor of $1/\eta$, leading to large statistical error.

One way to limit the increase in the variance is to allow for larger values of η by increasing the range of values of the forcing for which the nonlinear part of the response is sufficiently small. In theory, one can add an extra forcing to the physical perturbation of the system, called synthetic forcing, as long as this extra forcing preserves the invariant measure of the reference system. The aim is to find synthetic perturbations allowing to reduce the nonlinear part of the response as much as possible. In this talk, I will present a mathematical framework for quantifying the quality of synthetic forcings, in the context of linear response theory, and discuss various possible choices for them. I will illustrate my analysis with numerical results on the computation of the mobility in low dimensional systems.

Friday, July 22, 2022, 09:00 – 09:30, Lecture Hall 6

Hierarchical and adaptive methods for efficient risk estimation

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Financial derivatives in over-the-counter markets are subject to a series of valuation adjustments. These terms combine several layers of approximation, posing difficulties for efficient Monte Carlo estimation. As an example, we consider estimation of the value-at-risk of the credit valuation adjustment. This requires Monte Carlo estimation of

$$\mathbb{E}[\mathbb{H}(\mathbb{E}[f(\mathbb{E}[S_T \mid S_\tau]) \mid S_h])],$$

for a Lipschits function f, the Heaviside function $\mathbb{H}$ and relevant market and risk factors S at times h, τ and T. The nested structure of expectations, paired with numerical approximation of the market factors results in an $\mathcal{O}(\varepsilon^{-5})$ cost for standard Monte Carlo estimation with root mean square error ε. To remedy this, we construct a hierarchy of unbiased multilevel Monte Carlo estimators for $\mathbb{E}[f(\mathbb{E}[S_T \mid S_\tau]) \mid S_h]$, combined with adaptive multilevel Monte Carlo estimation for the expectation of the Heaviside function [1]. The resulting estimator has a greatly reduced $\mathcal{O}(\varepsilon^{-2}(\log \varepsilon)^2)$ cost.

[1] A.-L. Haji-Ali, J. Spence, and A. Teckentrup. Adaptive Multilevel Monte Carlo for Probabilities, 2021.

Thursday, July 21, 2022, 12:00 – 12:30, Lecture Hall 1

Convergence of the tamed Euler–Maruyama method for SDEs with discontinuous and polynomially growing drift

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Special session: Stochastic Computation and Complexity: Approximation of SDEs with Non-Standard Coefficients p.77

SDEs with irregular coefficients are currently of high interest. There are some specific types of irregularities leading to different problems when studying convergence of numerical schemes. These types of irregularities are usually studied separately in the literature. Examples are polynomially growing coefficients, or discontinuous coefficients. We consider SDEs that suffer from both of these types of irregularities and study strong convergence of the tamed Euler-Maruyama scheme.

Wednesday, July 20, 2022, 12:00 – 12:30, Lecture Hall 6

Multilevel Monte Carlo method with meta-model for advection-diffusion problems

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In this talk, we will present our results in modelling advection-diffusion processes using a combination of the multilevel Monte Carlo method (MLMC) and deep learning techniques. We deal with various simulations of Darcy flow and solute transport, particularly in the vicinity of a future underground nuclear waste repository. Our simulation problems are described by partial differential equations (PDEs) and solved numerically by the finite element method. Given the bedrock environment uncertainties, we consider simulation inputs as random variables and use the MLMC to estimate the expected values of simulation outputs. Depending on the required accuracy, it might lead to thousands of simulations, significantly affecting computational costs.

To overcome this difficulty, we substitute appropriate simulations with a meta-model. In particular, we employ a graph convolutional neural network (GCN) to approximate the solution of a PDE. This approach saves computational costs but also affects some MLMC estimator properties. The talk will cover the incorporation of a meta-model into a multilevel estimator, including its applicability and limitations. Numerical experiments will show the effectiveness of the proposed approach.

Thursday, July 21, 2022, 12:00 – 12:30, Lecture Hall 4

Dimension-independent Markov chain Monte Carlo on the sphere

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Special session: Advanced Particle Methods for Bayesian Inference p.50

We consider Bayesian analysis on high-dimensional spheres with angular central Gaussian priors. These priors model antipodally-symmetric directional data, are easily defined in Hilbert spaces and occur, for instance, in Bayesian binary classification and level set inversion. In this paper we derive efficient Markov chain Monte Carlo methods for approximate sampling of posteriors with respect to these priors. Our approaches rely on lifting the sampling problem to the ambient Hilbert space and exploit existing dimension-independent samplers in linear spaces. By a push-forward Markov kernel construction we then obtain Markov chains on the sphere, which inherit reversibility and spectral gap properties from samplers in linear spaces. Moreover, our proposed algorithms show dimension-independent efficiency in numerical experiments.

[1] H. C. Lie, D. Rudolf, B. Sprungk, T. J. Sullivan. Dimension-independent Markov chain Monte Carlo on the sphere. Preprint available at `https://arxiv.org/abs/2112.12185`

Monday, July 18, 2022, 12:00 – 12:30, Lecture Hall 4

Approximate Bayesian algorithm for tensor robust principal component analysis

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Special session: Developments in Markov Chain Monte Carlo p.56

Recently proposed Tensor Robust Principal Component Analysis (TRPCA) aims to exactly recover the low-rank and sparse components from their sum, extending the earlier Low-Rank Tensor Completion model representation. We construct a Bayesian approximate inference algorithm for TRPCA, based on regression adjustment methods suggested in the literature to correct for high-dimensional nature of the problem and sequential Monte Carlo approach with adaptive weights. Our results are compared to previous studies which used variational Bayes inference for matrix and tensor completion. In a short application, we study spatiotemporal traffic data imputation using nine-week spatiotemporal traffic speed data set of Guangzhou, China.

Friday, July 22, 2022, 09:30 – 10:00, Lecture Hall 1

Approximating distribution functions in uncertainty quantification using quasi-Monte Carlo methods

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Special session: Smoothing and Adaptive Methods p.75

As high-dimensional problems become increasingly prevalent in many applications, the effective evaluation of these problems within the limits of our current technology poses a great hurdle due to the exponential increase in computational cost as dimensionality increases. One class of strategies for evaluating such problems efficiently are quasi-Monte Carlo (QMC) methods. Recently the application of quasi-Monte Carlo methods to approximate expected values associated with solutions to elliptic partial differential equations with random coefficients in uncertainty quantification has been of great interest. In this talk, we look into extending this from the computation of expected values to the approximation of distribution functions by reformulating these functions as expectations of an indicator function. However this requires the integration of discontinuous functions and hence the need for preintegration, whereby we integrate out a single variable of the discontinuous function in order to obtain a function of one dimension less with sufficient level of smoothness to apply QMC methods. We also present some theoretical results regarding the error bounds associated with such approximations and the results of numerical experiments.

Thursday, July 21, 2022, 16:00 – 16:30, Lecture Hall 1

Using importance sampling to speed up non-intrusive uncertainty quantification for Monte Carlo simulations

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Monte Carlo (MC) methods are used in radiation therapy to simulate the transport and dose deposition of particles in patients. Additional uncertainty quantification (UQ) can be challenging, as a naive application of UQ methods, like (quasi-) MC or stochastic collocation, requires numerous dose computations at different points in the parameter space. We exploit that parametric uncertainties can be modelled through changes to the probability distributions describing non-deterministic input particle phase space for MC dose calculations. The concept of importance sampling can then be used to reconstruct unbiased estimators of the dose for different error realizations from the simulated particle trajectories of just one dose computation. Combined with regular non-intrusive strategies and multivariate uncertainty models, efficient estimates for quantities of interest such as the expected dose or dose variance, are obtained. Using the common assumption of Gaussian parameter distributions and uncertainty in the patient position, we further derive a parameter distribution for the direct reconstruction of the expected dose. For the variance, we choose a randomized quasi-MC approach and reconstruct the solution for each sample using the importance weighting approach. We achieve a speed-up of more than an order of magnitude while maintaining $99\% - 100\%$ agreement to a regular randomized quasi-MC reference for the dose expected value and variance according to the clinical $\gamma_{2mm/2\%}$-index, a distance to agreement criterion which is common in radiation therapy [1]. This contribution is based on [2].

[1] D. A. Low, W. B. Harms, S. Mutic, and J. A. Purdy. A technique for the quantitative evaluation of dose distributions. Medical Physics, 25(5):656661, May 1998.
[2] P. Stammer, L. Burigo, O. Jäkel, M. Frank, and N. Wahl (2022). Multivariate error modeling and uncertainty quantification using importance (re-) weighting for Monte Carlo simulations in particle transport. arXiv preprint arXiv:2202.02379.

Thursday, July 21, 2022, 18:00 – 18:30, Lecture Hall 4

Multi-Level Monte Carlo FEM for elliptic PDEs with Besov random tree priors

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Special session: Multilevel and Higher-Order Approximations for Stochastic Processes, Random Fields and PDEs p.63

We develop a Multilevel Monte Carlo (MLMC) FEM algorithm for linear, elliptic diffusion problems in polytopal domain $\mathcal{D} \subset \mathbb{R}^d$, with Besov-tree random coefficients. This is to say that the logarithms of the diffusion coefficients are sampled from so-called Besov-tree priors, which have recently been proposed to model data for fractal phenomena in science and engineering. Numerical analysis of the fully discrete FEM includes quadrature approximation and accounts for a) nonuniform pathwise upper and lower coefficient bounds, and for b) low path-regularity of the Besov-tree coefficients.

Admissible non-parametric random coefficients correspond to random functions exhibiting singularities on random fractals with tunable fractal dimension, but involve no a-priori specification of the fractal geometry of singular supports of sample paths. Optimal complexity and convergence rate estimates for quantities of interest are proved. A convergence analysis for MLMC-FEM is performed which yields choices of the algorithmic steering parameters for efficient implementation. A complexity ("error vs work") analysis of the MLMC-FEM approximations is provided.

Tuesday, July 19, 2022, 11:30 – 12:00, Lecture Hall 3

Logarithmic energy of points on $\mathbb{S}^2$

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Special session: Quantifying Notions of Equidistribution on the Sphere p.57

I will discuss a very classical problem: understanding the smallest possible logarithmic energy of n points $\{x_1, \ldots, x_n\} \subset \mathbb{S}^2$. It is not terribly difficult to see that one expects

$$\min_{\{x_1,\ldots,x_n\}} \sum_{\substack{i,j=1\\ i\neq j}}^{n} \log\left(\frac{1}{\|x_i - x_j\|}\right) \sim \left(\frac{1}{2} - \log 2\right) n^2 - \frac{n \log n}{2} + cn + o(n).$$

The constant c is expected to be

$$c_{\log} = 2\log 2 + \frac{1}{2}\log\frac{2}{3} + 3\log\frac{\sqrt{\pi}}{\Gamma(1/3)} \sim -0.055605\ldots$$

but so far only upper and lower bounds are known. I will explain a completely new approach to the problem that replaces the logarithm by something dramatically more complicated which will be dramatically easier to analyze – it gives rather sharp bounds on c and, assuming some local hexagonal symmetry, even predicts the (conjectured) optimal value. The same idea should be applicable to other manifolds.

Friday, July 22, 2022, 10:30 – 11:00, Lecture Hall 3

From numerical schemes for SDEs to analysis of Lipschitz maps

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Special session: Analysis and Simulation of SDEs in Non-Standard Settings. p.52

Various phenomena in insurance dividend optimization or in modeling the energy market lead to stochastic differential equations (SDEs) with discontinuous drift terms and degenerate diffusion. In real world applications, such drift terms are multidimensional, with discontinuities located at multidimensional manifolds. Numerical schemes and rates for such equations have been given in [3] and [4], requiring the points of discontinuity of the drift coefficient to be a smooth (C^4) manifold Θ. On the complement of this manifold, the drift is assumed to be smooth and thus locally Lipschitz continuous.

In [3], a transform was constructed, which transforms the SDE with discontinuous drift into one with Lipschitz continuous drift, thus allowing the application of classical results.

There, a key lemma was used that allows to conclude Lipschitz continuity of a function from its continuity plus 'intrinsic Lipschitz continuity'. However, the validity of this conclusion relies on the regularity of the manifold. In [2] we coined the notion of a permeable subset of a metric space and showed that permeability is a sufficient condition. In [1] we construct an impermeable Hölder-submanifold of $\mathbb{R}^d$ for which the conclusion fails to hold.

[1] Z. Buczolich, G. Leobacher, and A. Steinicke. Continuous functions with impermeable graphs. *arXiv:2201.02159*, 2022.

[2] G. Leobacher and A. Steinicke. Exception sets of intrinsic and piecewise Lipschitz functions. *Journal of Geometric Analysis*, 32, 2022.

[3] G. Leobacher and M. Szölgyenyi. A strong order 1/2 method for multidimensional SDEs with discontinuous drift. *Ann. Appl. Probab.*, 27(4):2383–2418, 2017.

[4] G. Leobacher and M. Szölgyenyi. Convergence of the Euler-Maruyama method for multidimensional SDEs with discontinuous drift and degenerate diffusion coefficient. *Numerische Mathematik*, 138(1):219–239, 2018.

Thursday, July 21, 2022, 15:30 – 16:00, Lecture Hall 1

Concave-Convex PDMP-based samplers

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Recently non-reversible samplers based on simulating piecewise deterministic Markov processes (PDMPs) have shown potential for efficient sampling in Bayesian inference problems. In this talk, I will show how these methods may be implemented efficiently when the rate function admits a concave-convex decomposition [1]. This approach facilitates simple implementation and computationally efficient thinning for a wide range of problems. In particular, our approach is well suited to local PDMP simulation where known conditional independence of the target can be exploited for potentially huge computational gains. I will show the merits of this approach with empirical scaling analysis and application to variable selection problems using reversible-jump PDMP-based samplers [2].

[1] Sutton, M., & Fearnhead, P. (2021). Concave-Convex PDMP-based sampling. In arXiv [stat.ME]. arXiv. http://arxiv.org/abs/2112.12897

[2] Chevallier, A., Fearnhead, P., & Sutton, M. (2020). Reversible Jump PDMP Samplers for Variable Selection. In arXiv [stat.CO]. arXiv. http://arxiv.org/abs/2010.11771

Thursday, July 21, 2022, 17:00 – 17:30, Lecture Hall 6

Component-by-component construction of randomized rank-1 lattice rules achieving almost the optimal randomized error rate

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Special session: Quasi-Monte Carlo Methods of High Order and Beyond p.68

We study a randomized quadrature algorithm to approximate the integral of periodic functions defined over the high-dimensional unit cube. Recent work by Kritzer, Kuo, Nuyens and Ullrich (2019) shows that rank-1 lattice rules with a randomly chosen number of points and good generating vector achieve almost the optimal order of the randomized error in weighted Korobov spaces, and moreover, that the error is bounded independently of the dimension if the weight parameters, γ_j, satisfy the summability condition $\sum_{j=1}^{\infty} \gamma_j^{1/\alpha} < \infty$, where α is a smoothness parameter. The argument is based on the existence result that at least half of the possible generating vectors yield almost the optimal order of the worst-case error in the same function spaces.

In this talk we provide a component-by-component construction algorithm of such randomized rank-1 lattice rules, without any need to check whether the constructed generating vectors satisfy a desired worst-case error bound. Similarly to the above-mentioned work, we prove that our algorithm achieves almost the optimal order of the randomized error and that the error bound is independent of the dimension if the same condition $\sum_{j=1}^{\infty} \gamma_j^{1/\alpha} < \infty$ holds.

Thursday, July 21, 2022, 17:30 – 18:00, Lecture Hall 6

Scaled lattice rules for integration over $\mathbb{R}^d$ achieving higher order convergence

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Special session: Quasi-Monte Carlo Methods of High Order and Beyond p.68

In this talk, we show that by simply scaling lattice rules from the unit cube $[0,1]^d$ to properly sized boxes on $\mathbb{R}^d$, taking into account all errors, we can achieve higher-order convergence in approximating an integral on $\mathbb{R}^d$ where the order of convergence matches the smoothness of the integrand function in a certain Sobolev space of dominating mixed smoothness. Our method only assumes that we can evaluate the integrand function f and does not assume a particular density nor the ability to sample from it. We also conduct numerical experiments comparing with other methods such as (i) direct product of Gauss–Hermite quadrature, (ii) Sparse grid based on Gauss–Hermite, and (iii) scaled interlaced Sobol' sequence. This talk is based on a join work with Dirk Nuyens [1].

[1] D. Nuyens and Y. Suzuki, *Scaled lattice rules for integration on $\mathbb{R}^d$ achieving higher-order convergence with error analysis in terms of orthogonal projections onto periodic spaces*, arXiv preprint `arXiv:2108.12639 [math.NA]`, (2021).

Thursday, July 21, 2022, 10:30 – 11:00, Lecture Hall 1

Existence, uniqueness, and approximation for jump-driven SDEs with discontinuous drift

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Special session: Stochastic Computation and Complexity: Approximation of SDEs with Non-Standard Coefficients p.77

In this talk we present an existence and uniqueness result of strong solutions to multi-dimensional jump-diffusion SDEs with discontinuous drift and general finite activity jumps. Jump-diffusion SDEs are used for example in models for applications in energy markets, where sudden movements of the energy price have to be captured. For a special scalar case, we study the strong convergence order of the Euler-Maruyama scheme and recover the optimal rate 1/2.

Thursday, July 21, 2022, 17:00 – 17:30, Lecture Hall 5

Option pricing and regularity of payoffs

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Special session: Simulation and Monte Carlo Methods in Quantitative Finance and Insurance p.74

We consider a problem of option pricing in a multi-variate financial market model from the perspective of quasi-Monte Carlo integration. For controlling the numerical approximation's error, the variation of the resulting integrand needs to be analyzed. In particular, we are able to show that a certain non-smooth payoff function leads to an integrand of bounded variation, even in the restrictive sense of Hardy and Krause. The key to this result is the application of a special transformation to the unit cube. The theoretical findings are illustrated by numerical examples and compared to results obtained using quantization techniques.

Monday, July 18, 2022, 12:00 – 12:30, Lecture Hall 6

Randomized quasi-Monte Carlo methods: Central limit theorem and confidence interval

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Quasi-Monte Carlo (QMC) methods are deterministic approximation methods to compute integrals by averaging the integrand taken at well-spread points of a *low discrepancy sequence*, but for which practical error bounds are rarely available. Randomized quasi-Monte Carlo (RQMC) methods have been introduced to cope with this problem. The type of RQMC method we focus on during this talk consists in randomizing the low-discrepancy sequence without losing its good repartition property and for which an error estimation is obtained by applying a central limit theorem over independent randomizations. To increase precision for a given computational budget, the number of independent randomizations is usually set to a small value so that a large number of points are used from each randomized low-discrepancy sequence to benefit from the fast convergence rate of quasi-Monte Carlo. This talk presents sufficient conditions on the relative growth rates of the number of randomizations and the quasi-Monte Carlo sequence length to ensure a central limit theorem and also an asymptotically valid confidence interval. We obtain several results based on the Lindeberg condition and expressed in terms of the regularity of the integrand and the convergence speed of the quasi-Monte Carlo method. We also analyze the resulting estimator's convergence rate.

The talk is based on the following papers:

[1] Nakayama M. K, Tuffin B. Sufficient conditions for a central limit theorem to assess the error of randomized quasi-Monte Carlo methods. In the *Proceedings of the 2021 Winter Simulation Conference* (IEEE), Phoenix, USA, December 2021.

[2] Nakayama, M. K., and B. Tuffin. Sufficient Conditions for Central Limit Theorems and Confidence Intervals for Randomized Quasi-Monte Carlo Methods. Techreport hal-03196085, INRIA. https://hal.inria.fr/hal-03196085. 2021

Wednesday, July 20, 2022, 12:00 – 12:30, Lecture Hall 5

Rare event estimation with PDE-based models

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Special session: Approximate Models for Rare Event Simulation and Uncertainty Quantification p.53

The estimation of the probability of rare events is an important task in reliability and risk assessment of critical societal systems, for example, groundwater flow and transport, and engineering structures. In this talk we consider rare events that are expressed in terms of a limit state function which depends on the solution of a partial differential equation (PDE). We present recent progress on mathematical and computational aspects of this problem: (1) the impact of the PDE approximation error on the failure probability estimate, and (2) the use of the Ensemble Kalman Filter for the estimation of failure probabilities.

Thursday, July 21, 2022, 10:30 – 11:00, Lecture Hall 3

On the power of function values for L_2-approximation

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Coauthor(s): Matthieu Dolbeault, David Krieg

Special session: Approximation from Random Data p.54

We survey on recent developments on L_2-approximation using function values. In particular, we explain how the individual contributions from [1,2,3,4] lead to the following statement: There is a universal constant $c > 0$ such that the sampling numbers of the unit ball F of every separable reproducing kernel Hilbert space are bounded by

$$g_{cn}(F)^2 \le \frac{1}{n} \sum_{k \ge n} d_k(F)^2,$$

where $d_k(F)$ are the Kolmogorov widths (or approximation numbers) of F in L_2. We also obtain similar upper bounds for more general classes, and provide examples where our bounds are attained up to a constant.
We also give pointers to other talks in this session, where different aspects of this problem will be discussed.

1 M. Dolbeault, D. Krieg and M. Ullrich, A sharp upper bound for sampling numbers in L_2, preprint.

2 D. Krieg and M. Ullrich, Function values are enough for L_2-approximation, *Found. Comput. Math.* **21** (2021), 1141–1151.

3 D. Krieg and M. Ullrich, Function values are enough for L_2-approximation: Part II, *J. Complexity* **66** (2021).

4 N. Nagel, M. Schäfer and T. Ullrich, A new upper bound for sampling numbers, *Found. Comput. Math.* **21** (2021).

Thursday, July 21, 2022, 15:30 – 16:00, Lecture Hall 4

Exact sequential inference for a diffusion-driven Cox process

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Temporal point processes are widely used to model phenomena in areas such as finance, epidemiology or signal processing. One general model is the sigmoidal Gaussian Cox process (SGCP), first introduced in Adams et al. (2009), where a transformation the intensity function governing the data-generation is assigned a Gaussian process prior. The resulting model posterior, however, is doubly-intractable with its likelihood function not having a closed form, and so various data-augmentation schemes are required to perform likelihood-based inference. We introduce a novel unbiased estimator of the SGCP likelihood, motivated by the thinning procedure used to generate non-homogeneous Poisson process realisations. The proposed estimator is a generalisation of the existing *Poisson estimator* of Wagner (1988) . By splitting the full observation window into smaller subintervals, a sequential Monte Carlo algorithm is used to perform exact inference on the intensity function, up to Monte Carlo error, with no need for data augmentation. Additionally, either a pseudo-marginal Markov chain Monte Carlo scheme or importance sampling can be used to sample from the hyper-parameter posteriors.

Friday, July 22, 2022, 09:30 – 10:00, Lecture Hall 6

Mobility estimation for Langevin dynamics using control variates

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The scaling of the mobility of two-dimensional Langevin dynamics in a periodic potential as the friction vanishes is not well understood for non-separable potentials. Theoretical results are lacking, and numerical calculation of the mobility in the underdamped regime is challenging because the computational cost of standard Monte Carlo methods is inversely proportional to the friction coefficient, while deterministic methods are ill-conditioned. In this talk, we propose a new variance-reduction method based on control variates for efficiently estimating the mobility of Langevin-type dynamics. We provide bounds on the bias and variance of the proposed estimator, and illustrate its efficacy through numerical experiments, first in simple one-dimensional settings and then for two-dimensional Langevin dynamics. Our results corroborate previous numerical evidence that the mobility scales as $\gamma^{-\sigma}$, where γ is the friction and $0 < \sigma \leq 1$, in the low friction regime and in the case of a simple non-separable potential.

Wednesday, July 20, 2022, 11:30 – 12:00, Lecture Hall 4

Unbiased approximation of posteriors via coupled particle Markov chain Monte Carlo

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Special session: Recent Advances in Unbiased Estimation Techniques p.72

Markov chain Monte Carlo (MCMC) is a powerful methodology for the approximation of posterior distributions. However, the iterative nature of MCMC does not naturally facilitate its use with modern highly parallel computation on HPC and cloud environments. Another concern is the identification of the bias and Monte Carlo error of produced averages. The above have prompted the recent development of fully ('embarrassingly') parallel unbiased Monte Carlo methodology based on coupling of MCMC algorithms. A caveat is that formulation of effective coupling is typically not trivial and requires model-specific technical effort. We propose coupling of MCMC chains deriving from sequential Monte Carlo (SMC) by considering adaptive SMC methods in combination with recent advances in unbiased estimation for state-space models. Coupling is then achieved at the SMC level and is, in principle, not problem-specific. The resulting methodology enjoys desirable theoretical properties. A central motivation is to extend unbiased MCMC to more challenging targets compared to the ones typically considered in the relevant literature. We illustrate the effectiveness of the algorithm via application to two complex statistical models: (i) horseshoe regression; (ii) Gaussian graphical models.

Tuesday, July 19, 2022, 16:00 – 16:30, Lecture Hall 1

A micro-macro Markov chain Monte Carlo method with applications in molecular dynamics

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In many problems and applications in molecular dynamics, one is typically interested in sampling from the time-invariant probability distributions of the system. Within many of these molecular systems, there is a natural time-scale separation present between the fast (microscopic) dynamics, and the slowly changing global conformation of the molecule determined by a few (macroscopic) variables.

Markov chain Monte Carlo (MCMC) is a general sampling algorithm that has been designed for sampling from probability distributions determined by a potential energy function. The objective is to construct a stochastic process whose time-invariant distribution is the invariant distribution of the molecular system By ergodicity, we can record samples from a single path of the process, and then these samples are consistent with invariant distribution. However, when the underlying system has a medium to large time-scale separation, the MCMC method may remain stuck in one of the local minima of the potential energy function, prohibiting a swift exploration of the complete state space of the molecular system.

In my talk, I will present a new micro-macro MCMC method (mM-MCMC) in which we first sample from the macroscopic variables, before reconstructing a new molecular instance that is consistent with the macroscopic value. I will give a detailed explanation of the algorithm, and show its efficiency on two molecular examples if time permits.

Wednesday, July 20, 2022, 14:30 – 15:00, Lecture Hall 1

Multilevel Markov Chain Monte Carlo for full-field data assimilation

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In recent years, the development of new observation techniques in various branches of engineering disciplines has created the possibility of generating full-field data on systems under study. An example of this is Digital Image Correlation in structural mechanics, which allows for full-field vibration measurements of civil engineering structures.

In some cases, however, the resolution of this full-field data is so high that the computational cost of using this data to solve Bayesian inverse problems becomes prohibitively expensive. While the incorporation of expensive forward models in a data assimilation context has recently been addressed by the multilevel Monte Carlo methodology, the standard setting still assumes that measurement data is only available in selected measurement points.

In this talk, we show a successful generalisation of a multilevel Markov Chain Monte Carlo algorithm, proposed by [1] within the context of structural health monitoring using full-field vibration data. The method reduces computational efforts by allowing the resolution of the data to vary across levels, along with the resolution of the forward model. We discuss our results from [2] and show that the data can be scaled in a simple way to decrease the cost of likelihood evaluation at the coarser levels.

[1] T.J. Dodwell, C. Ketelsen, R. Scheichl and A. Teckentrup. *Multilevel Markov Chain Monte Carlo*, SIAM Rev. 61(3):509-545, 2019.
[2] P. Vanmechelen, G. Lombaert and G. Samaey. *Multilevel Markov Chain Monte Carlo with likelihood scaling for full-field data assimilation in structural damage assessment*, in preparation.

Tuesday, July 19, 2022, 11:30 – 12:00, Lecture Hall 6

Zig-Zag for approximate Bayesian computation

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Special session: Recent Advances in Piecewise Deterministic Monte Carlo Methods p.71

Piecewise Deterministic Markov Processes (PDMPs) (see Fearnhead et.al.2018) have recently caught the attention of the MCMC community for having a non-diffusive behaviour and being able to explore the state space more efficiently. This makes them good candidates to generate MCMC algorithms. One important problem in Bayesian computation the last ten years is inference for models where the likelihood is intractable. A popular method to deal with problems in this setting is the Aprroximate Bayesian Computation (ABC). In this talk we describe a PDMP algorithm, based on the Zig-Zag process (see Bierkens and Roberts 2019), that is designed to target ABC posteriors. This way we combine the areas of PDMPs and ABC. We show that the algorithm targets the distribution of interest and we provide numerical examples to show its effectiveness. This is joint work with Richard Everitt.

References

[1] J. Bierkens, P. Fearnhead, and G. Roberts. The zig-zag process and super-efficient sampling for bayesian analysis of big data. Ann. Statist., 47(3):12881320, 06 2019. doi: 10.1214/18-AOS1715. URL https://doi.org/10.1214/18-AOS1715.

[2] R. Everitt and G. Vasdekis. ABC Zig-Zag. Under Preparation.

[3] P. Fearnhead, J. Bierkens, M. Pollock, and G. Roberts. Piecewise deterministic markov processes for continuous- time monte carlo. Statistical Science, 33, 11 2016. doi: 10.1214/18-STS648

Tuesday, July 19, 2022, 10:30 – 11:00, Lecture Hall 4

Optimal design of the Barker proposal and other locally-balanced Metropolis-Hastings algorithms

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Special session: Robust Innovations in Gradient-Based MCMC p.73

We study the class of first-order locally-balanced Metropolis-Hastings algorithms introduced in [1]. To choose a specific algorithm within the class the user must select a balancing function $g : \mathbb{R} \to \mathbb{R}$ satisfying $g(t) = tg(1/t)$, and a noise distribution for the proposal increment. Popular choices within the class are the Metropolis-adjusted Langevin algorithm (MALA) and the recently introduced robust alternative, the Barker proposal. We establish a universal limiting optimal acceptance rate of 57% and scaling of $n^{-1/3}$ as the dimension n tends to infinity among all members of the class under mild smoothness assumptions on g and when the target distribution for the algorithm is of the product form. In particular we obtain an explicit expression for the asymptotic efficiency of an arbitrary algorithm in the class, as measured by expected squared jumping distance. We optimise this expression under various constraints. We derive an optimal choice of noise distribution for the Barker proposal, optimal choice of balancing function under a Gaussian noise distribution, and optimal choice of first-order locally-balanced algorithm among the entire class, which turns out to depend on the specific target distribution. Numerical simulations confirm our theoretical findings and in particular show that a bi-modal choice of noise distribution in the Barker proposal gives rise to a practical algorithm that is consistently at least as efficient as MALA and as robust as the original version of the Barker proposal with Gaussian noise.

[1] Samuel Livingstone and Giacomo Zanella. The Barker proposal: combining robustness and efficiency in gradient-based MCMC. *Journal of the Royal Statistical Society: Series B (Statistical Methodology), in press, 2021.*

Thursday, July 21, 2022, 17:00 – 17:30, Lecture Hall 3

Schur's multiplication theorem and lower bounds for numerical integration

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Special session: Approximation from Random Data p.54

The classical Schur's product theorem says that the coordinate-wise product of two symmetric positive semi-definite matrices is a positive semi-definite matrix. We derive a new version of the Schur's product theorem and use it to solve an open problem of Erich Novak about the tractability of numerical integration in high dimensions. Furthermore, we show the consequences of the new Schur's theorem for Bochner's theorem, covariance matrices and mean values of trigonometric polynomials.

Tuesday, July 19, 2022, 17:30 – 18:00, Lecture Hall 6

Well-posedness of the MAP estimator in sequence spaces

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Special session: Laplace Approximation and Other Model-Based Preconditioning Methods for Monte Carlo Algorithms p.61

Many preconditioning methods rely on the existence of a "mode" or optimal point within the range of parameters around which to construct a region of special interest. For example, the Laplace approximation acts as a preconditioner which singles out (essentially) an elliptical region centered around the mode (i.e. point of highest density). In the context of Bayesian inversion, this mode is called the maximum-a-posteriori estimator (MAP estimator). While in finite dimensions, the MAP estimator is just the maximizer of the posterior density, it needs to be defined differently in infinite dimensional settings due to lack of a Lebesgue measure. We present new results regarding the well-posedness of this concept of "point of highest density" for parameter inference problems in sequence spaces ℓ^p with a diagonal Gaussian prior $\mu = \otimes N(0, \sigma_k^2)$. This includes and generalizes the case of parameter inference on arbitrary Hilbert spaces with a Gaussian prior.

Tuesday, July 19, 2022, 18:00 – 18:30, Lecture Hall 4

Comparison of Markov chains via weak Poincaré inequalities with application to pseudo-marginal MCMC

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Special session: Recent Advances in MCMC Sampling Techniques p.70

I will discuss the use of a certain class of functional inequalities known as weak Poincaré inequalities to bound convergence of Markov chains to equilibrium. We show that this enables the straightforward and transparent derivation of subgeometric convergence bounds for methods such as the Independent Metropolis–Hastings sampler and pseudo-marginal methods for intractable likelihoods, the latter being subgeometric in many practical settings. These results rely on novel quantitative comparison theorems between Markov chains. Associated proofs are simpler than those relying on drift and minorization conditions and the tools developed allow us to recover and further extend known results as particular cases. We are then able to provide new insights into the practical use of pseudo-marginal algorithms, such as analysing the effect of averaging in Approximate Bayesian Computation (ABC) and to study the case of lognormal weights relevant to Particle Marginal Metropolis–Hastings (PMMH).

[1] Andrieu, C., Lee, A., Power, S., Wang, A. Q. (2021). Comparison of Markov chains via weak Poincaré inequalities with application to pseudo-marginal MCMC. Preprint available at https://arxiv.org/abs/2112.05605.

Monday, July 18, 2022, 16:00 – 16:30, Lecture Hall 3

Optimal approximation of break-of-scale embeddings

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As a rule of thumb in approximation theory, the asymptotic speed of convergence of numerical methods is governed by the regularity of the objects we like to approximate. Besides classical isotropic Sobolev smoothness, the notion of dominating mixed regularity of functions turned out to be an important concept in numerical analysis. Although approximation rates of embeddings *within* the scales of isotropic or dominating-mixed L_p-Sobolev spaces are well-understood, not that much is known for embeddings *across* those scales. In this talk we introduce particular instances of new hybrid smoothness spaces which cover both scales as special cases. Moreover, we present (non-)adaptive wavelet-based approximation algorithms that achieve optimal dimension-independent rates of convergence for certain practically important break-of-scale embeddings.

References:

[1] G. Byrenheid, J. Hübner, and M. Weimar. Rate-optimal sparse approximation of compact break-of-scale embeddings. In preparation, 2022+.

Monday, July 18, 2022, 15:30 – 16:00, Lecture Hall 3

Covering numbers by intervals and equistribution theory

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Kronecker sequences belong to the classical examples of low-discrepancy sequences. From a dynamical viewpoint, they are realized as orbits of circle rotations by an irrational angle α. Moreover, the corresponding maps f_α are known to be dynamical systems of rank one. This means that there exist base sets B such that for arbitrarily high $h \in \mathbb{N}$ an arbitrarily large proportion of the circle can be covered by the Rokhlin tower $(f_\alpha^k(B))_{k=0}^{h-1}$. However, these sets B might be very complicated from a topological point of view. In this talk, we discuss how well topologically simple base sets B, i.e. unions of intervals, perform in covering the circle by a Rokhlin tower. We will also see how finding these simpler sets is related to the pair correlation statistic.

[1] C. Weiß. *Systems of rank one, explicit Rokhlin towers, and covering numbers.*to appear in: Arch. Math., 2021.

Friday, July 22, 2022, 10:00 – 10:30, Lecture Hall 1

A multilevel subset simulation for estimating rare events via shaking transformations

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Special session: Smoothing and Adaptive Methods p.75

In this talk, we analyse a multilevel version of subset simulation to estimate the probability of rare events for complex physical systems. Given a sequence of nested failure domains of increasing size, the rare event probability is expressed as a product of conditional probabilities. The proposed estimator uses different model resolutions and varying numbers of samples across the hierarchy of nested failure sets. The key idea in our proposed estimator is the use of a selective refinement strategy that guarantees the critical subset property which may be violated when changing model resolution from one failure set to the next. In order to estimate the probabilities of the underlying subsets we formulate and analyse a parallel one-path algorithm based on shaking transformations. Considering a physical model based on Gaussian transformation we can verify the ergodicity of the resulting Markov chain. Additionally, we present a detailed complexity analysis of the considered subset simulation.

Thursday, July 21, 2022, 17:30 – 18:00, Lecture Hall 5

Applications of the central limit theorem for pricing cliquet-style options

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Special session: Simulation and Monte Carlo Methods in Quantitative Finance and Insurance p.74

Cliquet-style options in different variants are basic building blocks in select products which are offered by German life insurance companies. We present both an analytical pricing approximation via the central limit theorem and a corresponding control variate Monte Carlo approach for their valuation. The control variate approach turns out to be a good alternative to the integral representation of [1]. Further, it can be modified to increase the efficiency of pricing cliquet-style options in the Heston price setting.

[1] Bernard, C., Li, W.V.: Pricing and hedging of cliquet options and locally-capped contracts. SIAM J. Fin. Math. 4, 353371, (2013)

Thursday, July 21, 2022, 11:30 – 12:00, Lecture Hall 5

Efficient importance sampling via stochastic optimal control for stochastic reaction networks

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Special session: Monte Carlo Methods and Variance Reduction Techniques for Stochastic Reaction Networks p.62

We explore the efficient estimation of statistical quantities, particularly rare event probabilities, for stochastic reaction networks and biochemical systems. To this end, we propose a novel importance sampling (IS) approach to improve the efficiency of Monte Carlo (MC) estimators when based on an approximate tau-leap scheme. The crucial step in the IS framework is choosing an appropriate change of probability measure for achieving substantial variance reduction. Typically, this is challenging and often requires insights into the given problem. Based on an original connection between finding the optimal IS parameters within a class of probability measures and a stochastic optimal control (SOC) formulation, we propose an automated approach to obtain a highly efficient path-dependent measure change. The optimal IS parameters are obtained by solving a variance minimization problem. We begin by deriving an associated backward equation solved by these optimal parameters. Given the challenge of analytically solving this backward equation, we propose a numerical dynamic programming algorithm to approximate the optimal control parameters. To mitigate the curse of dimensionality issue caused by solving the backward equation in the multi-dimensional case, we propose a learning-based method that approximates the value function using a neural network, the parameters of which are determined via a stochastic optimization algorithm. Our numerical experiments demonstrate that our learning-based IS approach substantially reduces the variance of the MC estimator. Moreover, when applying the numerical dynamic programming approach for the particular one-dimensional case, we obtained a variance that decays at a rate of $\mathcal{O}(\Delta t)$ for a step size of Δt, compared to $\mathcal{O}(1)$ for a standard MC estimator. For a given prescribed error tolerance, TOL, this implies an improvement in the computational complexity to become $\mathcal{O}(\mathrm{TOL}^{-2})$ instead of $\mathcal{O}(\mathrm{TOL}^{-3})$ when using a standard MC estimator.

[1] Hammouda, C. B., Rached, N. B., Tempone, R., & Wiechert, S. (2021). Optimal Importance Sampling via Stochastic Optimal Control for Stochastic Reaction Networks. arXiv preprint arXiv:2110.14335.

Thursday, July 21, 2022, 17:30 – 18:00, Lecture Hall 3

A randomised lattice algorithm for integration using a fixed generating vector

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Special session: Approximation from Random Data p.54

This talk will focus on a new randomised algorithm for lattice-based integration. In [1], it was shown that there exists a randomised algorithm producing a lattice rule which gives the optimal rate of convergence for the worst-case expected error and in [2], it was shown that this rate can be achieved with a constructible randomised algorithm. These two algorithms involve choosing both the generating vector and the number of sample points at random. In this talk we will see that, with a carefully selected generating vector, only the number of sample points need be chosen at random in order to achieve the optimal rate of convergence for the worst-case expected error.

[1] P. Kritzer, F. Y. Kuo, D. Nuyens, M. Ullrich "Lattice rules with random n achieve nearly the optimal $O(n^{-\alpha-1/2})$ error independently of the dimension." *Journal of Approximation Theory* 240 (2019): 96-113.

[2] J. Dick, T. Goda, K. Suzuki "Component-by-component construction of randomized rank-1 lattice rules achieving almost the optimal randomized error rate." *preprint* (2021)

Friday, July 22, 2022, 10:30 – 11:00, Lecture Hall 5

Pseudorandom sequences derived from automatic sequences

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Special session: Pseudo-Random Number Generation. p.65

Many automatic sequences, such as the Thue-Morse sequence or the Rudin-Shapiro sequence, have some desirable features of pseudorandomness such as a large linear complexity and a small well-distribution measure. However, they also have some undesirable properties in view of certain applications. For example, the majority of possible binary patterns never appears in automatic sequences and their correlation measure of order 2 is extremely large.

Certain subsequences, such as automatic sequences along squares, may keep the good properties of the original sequence but avoid the bad ones.

In this survey talk we investigate properties of pseudorandomness and non-randomness of automatic sequences and their subsequences and present results on their behaviour under several measures of pseudorandomness including linear complexity, correlation measure of order k, expansion complexity and normality.

[1] L. Mérai, A. Winterhof, Pseudorandom sequences derived from automatic sequences, Cryptogr. Commun., to appear, https://arxiv.org/abs/2105.03086.

Monday, July 18, 2022, 11:30 – 12:00, Lecture Hall 6

Which problems can be solved by randomized algorithms?

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Let F and G be separable Banach spaces. A linear problem is given by a continuous linear operator $S : F \to G$. The aim ist to approximate $S(f)$ for each $f \in F$ by means of an algorithm. Approximation error of an algorith A is given by

$$e^{det}(A,S) = \sup_{f \in F, \|f\|_F = 1} \|S(f) - A(f)\|_G \quad \text{if } A \text{ is a deterministic algorithm}$$

and

$$e^{ran}(A,S) = \sup_{f \in F, \|f\|_F = 1} \mathbb{E}\left[\|S(f) - A(\omega, f)\|_G\right] \quad \text{if } A \text{ is a randomized algorithm.}$$

Denote by $e^{\text{det}}(n,S)$ the minimal error of any deterministic algorithm using at most n information evaluation. We say that the problem S is solvable in the deterministic setting when

$$\lim_{n \to \infty} e^{det}(n,S) = 0.$$

We define $e^{ran}(n,S)$ analogously and say that the problem S is solvable in the randomized setting if

$$\lim_{n \to \infty} e^{ran}(n,S) = 0.$$

In this talk we focus on the situation when we can use any continuous functional on F as an information.

The main question is: which problems are solvable? It is well-known that in the deterministic setting the problem given by S is solvable if and only if S is a compact operator. The situation seems to be more complicated if we allow for randomized algorithms. In this talk we sketch the proof that if the operator S is not finitely strictly singular then it is certainly not solvable in the randomized setting. Furthermore, we present an example demonstrating that the proof technique used cannot be succesfully applied to show that only compcat operators are solvable in the randomized setting. In the end we present some open questions.

Thursday, July 21, 2022, 16:00 – 16:30, Lecture Hall 4

Analysis and optimization of certain parallel Monte Carlo methods in the low temperature limit

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Coauthor(s): Paul Dupuis

Metastability is a formidable challenge to Markov chain Monte Carlo methods. In this talk we present methods for algorithm design to meet this challenge. The design problem we consider is temperature selection for the infinite swapping scheme, which is the limit of the widely used parallel tempering scheme obtained when the swap rate tends to infinity. We use a recently developed tool for the large deviation properties of the empirical measure of a metastable small noise diffusion to transform the variance reduction problem into an explicit graph optimization problem. The nodes in the graph optimization problem correspond to metastable states of the noiseless dynamics. Our first analysis of the optimization problem is in the setting of a double well model, and it shows that the optimal selection of temperature ratios is a geometric sequence except possibly the highest temperature. In the same setting we identify two different sources of variance reduction, and show how their competition determines the optimal highest temperature. In the general multi-well setting we prove that the same geometric sequence of temperature ratios as in the two-well case is always nearly optimal, with a performance gap that decays geometrically in the number of temperatures. Moreover, this optimal placement of temperatures is explicit and independent of the particular functional being integrated on the potential.

[1] P. Dupuis, G.-J. Wu (2022) Analysis and optimization of certain parallel Monte Carlo methods in the low temperature limit, *SIAM Journal Multiscale Modeling and Simulation*, Vol 20, 220–249.

[2] P. Dupuis, G.-J. Wu (2021) Large deviation properties of the empirical measure of a metastable small noise diffusion, *Journal of Theoretical Probability.*

[3] P. Dupuis, Y. Liu, N. Plattner and J. D. Doll (2012) On the infinite swapping limit for parallel tempering, *SIAM Journal Multiscale Modeling and Simulation*, Vol 10, 986–1022.

Tuesday, July 19, 2022, 16:00 – 16:30, Lecture Hall 5

Managing the risk of derivatives underlying portfolios

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Derivatives underlying a portfolio is popular on the market to diversify the market risk. However, existing method, the nested simulation, is quite time-consuming for pricing and managing the risk. In this article, we propose an efficient approach, randomized willow tree method. There are three main stages for our approach, portfolio distribution approximation, randomized willow tree construction and managing the risk of derivatives. We first generate some simulated paths to describe the evolution of dynamic portfolio values. Then, the minimal relative entropy (MRE) method is applied to approximate the distribution of portfolio values at each time based on the simulated data. After the approximated distributions are determined, a randomized willow tree can be constructed for pricing and managing the risk of derivatives underlying the portfolio. Finally, we apply the proposed approach to calculate annual dollar delta, 99% VaR and CVaR of a particular derivative, i.e., a 19-year variable annuity with guarantee riders. This application demonstrates the efficiency and accuracy of the proposed approach compared with the common nested simulation technique, especially for a large pool of derivatives underlying the same portfolio.

Tuesday, July 19, 2022, 15:30 – 16:00, Lecture Hall 1

Stereographic Markov chain Monte Carlo

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Coauthor(s): Krzysztof Łatuszyński and Gareth O. Roberts

High dimensional distributions, especially those with heavy tails, are notoriously difficult for off the shelf MCMC samplers: the combination of unbounded state spaces, diminishing gradient information, and local moves, results in empirically observed ”stickiness” and poor theoretical mixing properties – lack of geometric ergodicity. In this talk, we introduce a new class of MCMC samplers that map the original high dimensional problem in Euclidean space onto a sphere and remedy these notorious mixing problems. In particular, we develop random-walk Metropolis type algorithms as well as versions of Bouncy Particle Sampler that are uniformly ergodic for a large class of light and heavy tailed distributions and also empirically exhibit rapid convergence in high dimensions.

Wednesday, July 20, 2022, 12:00 – 12:30, Lecture Hall 4

Multi-index sequential Monte Carlo and randomized multi-index sequential Monte Carlo ratio estimators

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Coauthor(s): Kody J.H. Law, Xinzhu Liang

Special session: Recent Advances in Unbiased Estimation Techniques p.72

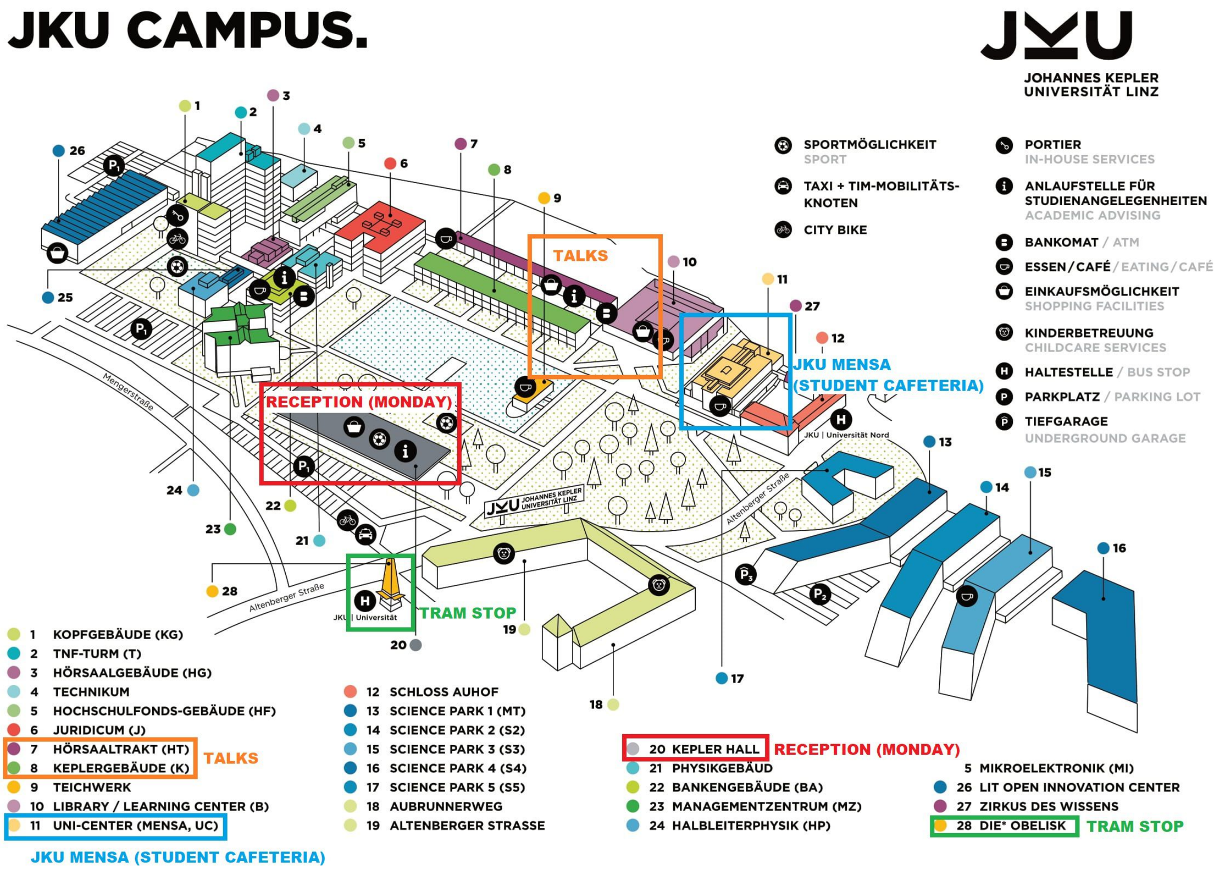
We consider the problem of estimating expectations with respect to a target distribution with an unknown normalizing constant, and where even the unnormalized target needs to be approximated at finite resolution. This setting is ubiquitous across science and engineering applications, for example in the context of Bayesian inference where a physics-based model governed by an intractable partial differential equation (PDE) appears in the likelihood. A multi-index sequential Monte Carlo (MISMC) method and a randomised multi-index sequential Monte Carlo method are used to construct ratio estimators which provably enjoy the complexity improvements of multi-index Monte Carlo (MIMC) as well as the efficiency of Sequential Monte Carlo (SMC) for inference. The ratio estimators are constructed by the ratio of two unbiased estimators of the corresponding unnormalised targets. This introduces discretisation bias to MISMC method, but the partially unbiased formulation offers the theoretical evidence of convergence under realistic assumptions. By leveraging a randomisation strategy as randomised MISMC, the bias can be removed entirely, which simplies estimation substantially. Both of the proposed methods provably achieve the canonical complexity of MSE^{-1}, while single level methods require $\mathrm{MSE}^{-\xi}$ for $\xi > 1$. This is illustrated on examples of Bayesian inverse problems with an elliptic PDE forward model in 2 spatial dimensions, where ξ is $3/2$. It is also illustrated on a more challenging log Gaussian Cox model from spatial statistics, where single level complexity is approximately $\xi = 9/4$ and multilevel Monte Carlo (or MIMC with an inappropriate index set) gives $\xi = 5/4 + \omega$, for $\omega > 0$, whereas our methods are again canonical.

Practical Information

Conference Venue and Important Dates

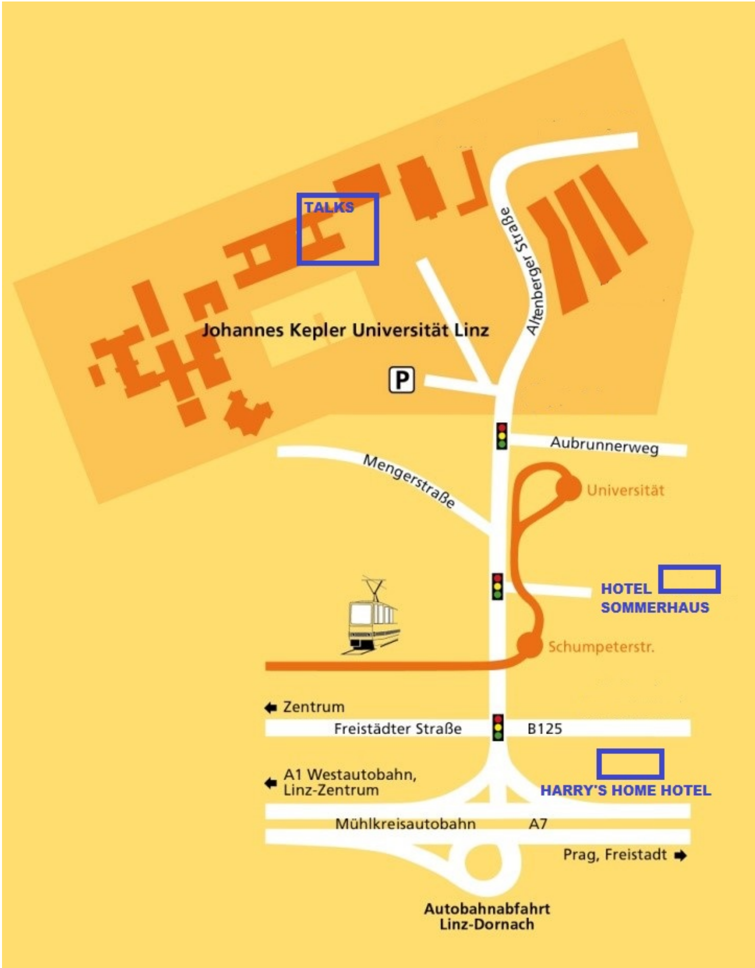
The conference is hosted by the Johannes Kepler University (JKU) Linz and the Austrian Academy of Sciences, on the campus of JKU. All talks will take place in Lecture Halls 1, 3, 4, 5, or 6, which are located in the Lecture Hall Wing (Lecture Hall 1, "Hörsaaltrakt, HT") or the Kepler Building (Lecture Halls 3–6, "Keplergebäude, K"). The two buildings are connected to each other and located next to the JKU Library, close to the pond.

The German word for Lecture Hall is "Hörsaal", sometimes abbreviated "HS".



Approximate location of Sommerhaus and Harry's Home

The map below should give you a good idea of the locations of the two main conference hotels ("Sommerhaus" and "Harry's Home") and where they are located. It will take approximately 15 minutes to walk to the Lecture Halls from Hotel Sommerhaus and about 20 minutes from Harry's Home Hotel.



Conference Schedule

The conference schedule will be printed in the program book, and will be available online at the conference webpage. The online version of the schedule will be kept as much up-to-date as possible, reflecting also short-term changes.

Registration and Information Desk

The registration and information desk is located outside of Lecture Hall 1, in Hall B ("Halle B"). Sunday afternoon registration will take place from 13:30 to 16:00 on July 17. Monday morning registration will take place from 08:00 to 12:30 on July 18. In addition, there will be staff at the information desk during the breaks if you should have any questions or concerns.

Sunday Tutorials

Sunday afternoon tutorials will be held in Lecture Hall 1, and are given by Frances Y. Kuo (14:15–15:45) and Chris J. Oates (16:00–17:30).

Opening Ceremony

The opening ceremony will be held in Lecture Hall 1 on Monday, July 18, at 08:45, before the first plenary talk.

Plenary Talks

Plenary talks will be held in Lecture Hall 1. Plenary talks are 50 minutes long, plus 10 minutes for questions and discussions. Due to the tight conference schedule, we kindly ask the chairs to strictly observe the time constraints.

All other talks

All other talks (except plenary talks and tutorials) will be held in parallel sessions in Lecture Halls 1,3,4,5, and 6. These talks are 25 minutes long plus 5 minutes for questions and discussions. Due to the tight conference schedule, we kindly ask all speakers and chairs to strictly observe the time constraints.

Coffee Breaks

Morning and afternoon coffee breaks will take place outside of Lecture Hall 1 in Halls B and C ("Halle B" and "Halle C").

Reception (Monday)

On Monday, July 18, there will be a welcome reception from 18:30 to 20:30. Drinks and finger food will be provided at the Kepler Hall building (across the road from the university tram stop). Please note that all participants (conference participants and accompanying persons) must be registered in advance for this event.

Award Ceremony of the Journal of Complexity (Tuesday)

On Tuesday, July 19, there will be a short ceremony to award IBC Awards and IBC Young Researcher Awards of the Journal of Complexity. The ceremony will be chaired by the Chief Editor of the journal, Erich Novak, and takes place at 13:50 in Lecture Hall 1 (immediately before the afternoon plenary talk).

Editorial Board Meeting of the Journal of Complexity (Tuesday)

On Tuesday, July 19, the members of the Editorial Board of the Journal of Complexity will have a closed meeting at 19:00. If you have any comments or suggestions regarding the journal, please approach any member of the Editorial Board prior to this meeting. The meeting will take place at RICAM, in the Science Park 2 Building on campus (Science Park 2, Floor 4, Room 416-2, RICAM's "bigger" seminar room).

Conference Photo (Wednesday)

A conference photo will be taken on Wednesday, July 20, at 16:30, right after the afternoon plenary talk. Details will be announced during the opening of the conference.

Conference Dinner (Wednesday)

The conference dinner will take place at the restaurant "Stadtliebe" in Linz, located in the city center on Landstraße 31. There is a direct tram connection between the campus of JKU Linz and the location of the restaurant (take Lines 1 or 2 and get off at "Mozartkreuzung").

Please note that all participants (conference participants and accompanying persons) must be registered in advance for this event. Wristbands for entering the restaurant will be handed out to all registered participants and accompanying persons.

Steering Committee Meeting (Thursday)

On Thursday, July 21, the MCQMC Steering Committee will have a closed meeting, starting at 19:00. If you have any comments or suggestions, or would like to propose hosting a future conference, please approach any member of the Steering Committee prior to this meeting. The meeting will take place in the "Teichwerk" restaurant, located on the pond of the JKU campus.

Covid-19 Rules

The Covid-19 situation has relaxed considerably over the past months in most of Europe, but there are a few Covid rules that we kindly ask you to observe.

- Even though there is no strict mask mandate on JKU campus any longer, there is a strong recommendation to wear masks in crowded places. We fully support this recommendation and ask you to **wear masks** whenever you are within larger groups of people. **Every conference participant will find an FFP2 mask in their conference kit. Please use it.**

- Should you suspect that you might have contracted Covid-19, please **do not** come to the conference venue **under any circumstances**, but make yourself known to the conference organizers. Call the Austrian Agency for Health at +43-732-1450, where you will be assisted with organizing a PCR test and all further steps.

- If you should show symptoms typical of Covid-19 but are not sure whether you might have Covid or a cold or flu, **do not** come to the conference until you have a negative PCR test result.

- In any case, please use common sense, and try to help us in keeping MCQMC 2022 Covid-19 free.

Food

Lunch will *not* be provided. A convenient and inexpensive place to have lunch during the conference week is JKU Mensa, which is the main student cafeteria, located close to the lecture halls, next to the JKU library (see also the campus map). Furthermore, there are several cafes and restaurants on and close to the campus. Please see the table and the map below.

1A	**JKU Mensa**	`www.mensen.at`	Mon–Fri	11:00–13:30
1B	**Cafe Ch@t**	Keplergebäude	Mon–Thu Fri	08:00–19:00 08:00–14:00
1C	**Science Cafe**	Science Park 3	Mon–Thu Fri	08:00–16:00 08:00–14:00
1D	**Cafe Sassi**	Bankengebäude `www.sassi.at`		Temporarily closed.
1E	**Teichwerk**	University pond `www.dasteichwerk.at`	Mon–Thu Fri	08:00–16:00 08:00–14:00
2	**KHG Mensa**	Mengerstr. 23 `https://www.dioezese-linz.at/khg/mensa/menueplan`	Mon–Fri	11:00–13:00
3	**Winklermarkt** (Supermarket & Restaurant)	Altenbergerstr. 40 `https://winklermarkt.at/menuplan/`	Mon–Thu Fri Sat	07:30–18:30 07:30–19:00 07:30–17:00
4a	**Pizzeria Bella Casa**	Aubrunnerweg 1a Phone: +43-732-245646	Mon–Sun	11:00–15:00 17:00–24:00
4b	**Chinese Restaurant Jadegarten**	Aubrunnerweg 11 Phone: +43-732-750160	Mon–Sun	11:00–14:30 17:00–23:00
5	**Restaurant Burgerista**	Altenbergerstr. 6–8 Phone: +43-50-666666	Mon–Thu Fri–Sat Sun	10:30–22:00 10:30–23:00 10:30–23:00
6	**Restaurant Peter's Platz**	Freistädter Str. 297 Phone: +43-732-251112	Mon–Sat Sun	11:00–23:00 11:00–17:00
7	**Subway**	Freistädter Str. 313	Mon–Sun	11:00–22:00
8	**Asian Restaurant Ost18**	Freistädter Str. 315 Phone: +43-732-244042	Tue Wed–Mon	11:30–14:30 11:30–14:30 17:30–23:00
9	**Raab Mensa** (Restaurant & Bar)	Julius-Raab-Str. 10 Phone: +43-732-24570 `www.sommerhaus-hotel.at/de/linz#speiseplan`	Bar: Mon–Thu Sat–Sun Restaurant: Mon–Sun	 06:30–23:30 06:30–11:00 11:30–14:30 17:00–21:00
10	**McDonald's & McCafe**	Freistädter Str. 298	Sun–Thu Fri–Sat	07:00–00:00 07:00–02:00
11	**"Penny"** (Supermarket)	J.W.-Klein-Str. 58	Mon–Fri Sat	07:40–20:00 07:40–18:00
12	**"Hofer"** (Supermarket)	Freistädter Str. 401	Mon–Fri Sat	07:40–20:00 07:40–18:00
13	**"Billa"** (Supermarket)	Freistädter Str. 400	Mon–Fri Sat	07:40–20:00 07:40–18:00
14	**"Spar"** (Supermarket)	Altenbergerstr. 69 (on JKU campus)	Mon–Fri Sat	07:30–19:45 08:00–18:00

Travel to Linz

Linz is the third-largest city of Austria, located on the river Danube in the northern part of the country, about half-way between Vienna and Salzburg.

Linz main station ("Linz Hauptbahnhof") can be easily reached from the airports of Vienna, Munich, and Salzburg, and via fast train connections from other European cities. In particular, there is a direct train connection between Vienna airport and Linz main station that takes approximately 1 hour and 40 minutes, departing from Vienna airport every hour during daytime. For details on train connections see `https://www.oebb.at/en`

Arriving at the main station, you can reach the campus of JKU Linz and the conference hotels by taking Trams 1 or 2 to "JKU/Universität" and getting off at the last stop; this takes approximately 25 minutes. If you stay in Hotel Sommerhaus or Harry's Home, it may be more convenient to get off at the stop "Schumpeterstraße". Trams leave on the underground level of the main station. You can buy tickets from the ticket machines at the platform or at newsagents/tobacco stores ("Trafik"). In the latter case, please do not forget to validate your ticket at the ticket machine before getting on the tram. Alternatively, you can download the `LinzMobil` app, where you can plan your trip and buy tickets online.

Linz also has a smaller airport with connections to other European airports. If you arrive at Linz airport, you have the following options to go to the conference venue.

- Take Bus 601 to the main station (approx. 20 minutes), and continue from there by tram (approximately 25 minutes, see above).
- Shuttle service:

  `https://www.linz-airport.com/en/Passengers-Visitors/To-and-from-Linz/Airport-Shuttle`.
- Taxi (approx. 45–50 EUR).

Should you arrive by car, the easiest way to reach the JKU campus is to take "A7/Mühlkreis-autobahn" to the exit "Linz-Dornach". Please note that parking is rather limited on the campus of JKU.

Public transport in Linz

Public transport in Linz is based on trams and buses. Trams 1 and 2 offer a direct connection between the city center and the conference venue. For general information about public transport in Linz, including timetables and maps, visit the "Linz AG Linien" webpage, `https://services.linzag.at/efa/index-en.jsf#`.

An easy way to plan trips and buy tickets for public transport online is to download the `LinzMobil` app.

If you need a taxi, please call +43-732-6969 or contact the conference desk. We can order a taxi for you.

Equipment in Lecture Halls

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

We strongly encourage you to make yourself known to your session chair and (if necessary) the MCQMC staff member assigned to your lecture room, prior to your talk. Please bring your talk in the form of a PDF document on a USB storage device and make sure that your talk is copied onto the desktop computer during the break prior to your talk. We cannot guarantee that other file formats than PDF can be displayed correctly.

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

Internet and Computer Access

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

If you cannot use eduroam, you will be granted access to the JKU wireless network on campus. You will be asked at the registration desk whether you need an account for the JKU wireless network or not; if you would like to make use of this service (and not use eduroam), you will have to sign that you agree to the terms of service. You can find these at

`https://www.jku.at/fileadmin/gruppen/61/Satzung___Co/Betriebs-_und_Benuetzungsordnung_ZID/Betriebs-_und_Benuetzungsordnung_ZID.pdf`

A printed version (in German) will be displayed at the registration desk.

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

Printing and Photocopying

The main library of JKU offers the possibility to print, copy, and scan for guests; you will have to pay a fee. All further information can be obtained from the main desk of the JKU library.

Alternatively, conference organizers may be willing to help you with a small amount of printing or photocopying. We ask for your understanding, though, that we cannot provide this as a regular service, but only in exceptional cases.

Useful Contacts and Services on Campus

In case of emergencies, here are a few useful phone numbers:

- Fire department: 122
- Police: 133
- Medical emergencies: 144
- Emergency calls at the University campus: 8144 (for urgent cases), otherwise: 9100
- Europe-wide general emergency call: 112
- Information about physicians on duty after hours: 141

Note that the Europe-wide general emergency number 112 can be called from any cell phone even without a valid subscription or prepaid SIM card inserted.

Physicians, Hospitals, and Pharmacies

The following physicians are located in the area of Hotel Sommerhaus and the campus.

Dr. Winfried Mraczansky	Altenbergerstr. 43 4040 Linz Phone: +43-732-245655	Mon Tue, Thur Wed Fri	08:00–11:30, 16:00–17:30 08:00–11:30 08:00–11:30, 16:00–17:30 08:00–11:00
Dr. Dieter Mojzischek	Streimlingweg 3 4040 Linz Phone: +43-732-251600	Mon–Fri	by appointment
Dr. Gottfried Jetschgo	Pulvermühlstr. 23 4040 Linz Phone: +43-732-254121	Mon Tue–Fri Tue, Thu	08:00–12:00 08:00–11:00 16:00–18:00

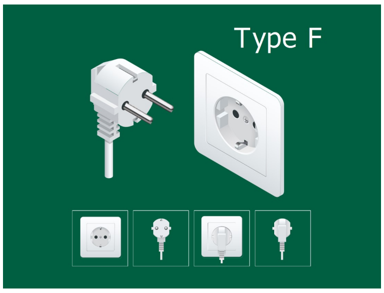
Should you need medication the doctor will give you a prescription which you can take to any pharmacy to pick up the medicine. Pharmacies are also the only places which sell over-the-counter drugs like painkillers, etc. The pharmacy closest to the campus is located in the building of "Winklermarkt" (Altenbergerstr. 40). After hours and on weekends, there are signs in all pharmacies to inform you about the nearest pharmacy on duty. This information can also be found online at

`https://apo24.at/apotheken/nachtdienste/oberoesterreich/95/linz/`.

The general hospital in Linz is Allgemeines Krankenhaus (AKH Linz), Krankenhausstraße 9, which also has an emergency room. In addition, Linz has a number of specialized hospitals, some of which also have emergency rooms. In the case of a medical emergency, call 144.

Power Plugs in Austria

Power sockets are of Type F, standard voltage 230 V, standard frequency 50 Hz.



Closing of the Conference

MCQMC 2022 will be closed with a few short announcements and remarks immediately after the final plenary lecture which finishes at 12:30 on Friday, July 22, in Lecture Hall 1. There will also be a short presentation about MCQMC 2024.

Proceedings

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

The submission deadline for manuscripts is December 31, 2022. Please send your submissions as a pdf file to `mcqmc2022@ricam.oeaw.ac.at`.

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

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