جامعة الملك عبدالله للعلوم والتقنية
King Abdullah University of Science and Technology

Center for Uncertainty Quantification

Advances in Uncertainty Quantification Methods, Algorithms and Applications (UQAW 2016)

January 5 - 10, 2016
8:30 a.m. - 6:30 p.m.

WORKSHOP TOPICS

1- Uncertainty Quantification Methods and Algorithms
2- Verification and Validation
3- Experimental Design
4- Applications to Problems in Computational Science, Engineering, Networks and the Environment

ORGANIZERS

RAUL TEMPONE
Director Center for Uncertainty Quantification in Computational Science & Engineering
Professor, Computer, Electrical and Mathematical Sciences and Engineering Division, KAUST

OMAR KNIO
Deputy Director, Center for Uncertainty Quantification in Computational Science & Engineering
Professor, Computer, Electrical and Mathematical Sciences and Engineering Division, KAUST

For more information visit:
http://sri-uq.kaust.edu.sa

Or contact:
SRI.UQ@KAUST.EDU.SA

Welcome from the Directors of KAUST SRI Center for Uncertainty Quantification in Computational Science and Engineering

On Behalf of SRI Center for Uncertainty Quantification in Computational Science and Engineering, we are delighted to welcome you to KAUST, and to 4th annual meeting of the Center, *Advances in Uncertainty Quantification Methods, Algorithms and Applications* (UQAW2016), January 5-10, 2016 at KAUST in Thuwal, KSA.

First and foremost, we wish to thank the Advisory Board members who have accepted to join us for this meeting, along with all the attendees, and of course of the Thrust Leaders and the team members.

This fourth annual meeting is intended to report on the latest advances and innovations in Uncertainty Quantification Methods, Algorithms and Applications (UQAW 2016); as well as serve as a discussion forum for exchanging information about the development, application, and experimental results by bringing together researchers, academics, and students working in the field.

It is with great pleasure that we present these proceedings of abstracts and posters. The annual meeting is very successful with over 75 contributions (as oral or poster presentations) together with 20 invited talks delivered from authors of the Center and from diverse international affiliations (e.g. United States, Germany, Canada, France, Greece, UK, and others). By organizing UQAW 2016, it is our sincere hope to help promote and broaden the diffusion of the research activities in the Uncertainty Quantification field.

We would like to express our sincere appreciation to the staff and to colleagues who participate in the workshop.

KAUST, December 2015 *Raúl Tempone and Omar Knio*

جامعة الملك عبدالله للعلوم والتقنية
King Abdullah University of Science and Technology

Center for Uncertainty Quantification

Advances in Uncertainty Quantification Methods, Algorithms and Applications (UQAW 2016)

January 5 – 10, 2016
8:30 a.m. – 6:30 p.m.

	TUESDAY, JANUARY 5	WEDNESDAY, JANUARY 6	THURSDAY, JANUARY 7	FRIDAY, JANUARY 8	SATURDAY, JANUARY 9	SUNDAY, JANUARY 10
7:00–8:00 a.m.						**Breakfast external visitors**
7:45 a.m.				Bus to KAEC	Bus to KAEC	
8:00-8:30 a.m.	**Light Breakfast** & Welcome Registration	**Light Breakfast**	**Light Breakfast**	**Breakfast external visitors**	**Breakfast external visitors**	Bus to KAUST
8:30-8:45 a.m.	KAUST CEMSE Dean Opening Speech					
	Chair: Christian Bayer	Chair: Omar Ghattas	Chair: Raul Tempone	Chair: Frances Kuo	Chair: Omar Knio	
8:45-9:45 a.m.	Frances Kuo	Omar Knio	Tiejun Li	Raul Tempone	Fabio Nobile	
9:45-10:15 a.m.	Dirk Nuyens	Christian Bayer	Omar Ghattas	Aretha Teckentrup	Ibrahim Hoteit	
10:15-10:45 a.m.	Habib Najm	Olof Runborg	Anthony Nouy	Erik von Schwerin	Matteo Icardi	
10:45-11:00 a.m.	**Coffee Break**	**Coffee Break**	**Coffee Break**	**Coffee Break**	**Coffee Break**	
11:00-11:30 a.m.	Lorenzo Tamellini	Claudia Schillings	Ankit Gupta	Haakon Hoel	Olivier Le Maitre	Local Activities: Snorkeling
11:30 a.m.-12:00 p.m.	Ahmad Rushdi	Markus Siebenmorgen	Pedro Vilanova	Martin Eigel	Serge Prudhomme	
12:00-12:30 p.m.	Ajay Jasra	Mattias Sandberg	Gerardo Rubino	Abdul Lateef Haji Ali	Alexander Litvinenko	
12:30-2:00 p.m.	**Lunch**	**Lunch**	**Lunch**	**Lunch**	**Lunch**	
	Chair: Habib Najm	Chair: Olivier Le Maitre		Chair: Bani Mallick	Chair: Serge Prudhomme	
2:00-2:30 p.m.	Nuutti Hyvönen	Kody Law		Quan Long	Bani Mallick	
2:30-3:00 p.m.	Giovanni Migliorati	Mohamed Ebeida	Bus to KAEC for external visitors	Marco Scavino	Diogo Gomes	
3:00-3:30 p.m.	Hermann Matthies	Khaled Ben Letaief		Ben Mansour Dia	Ricardo Lima	Bus to KAEC
3:30-4:00 p.m.	**Coffee Break**	**Coffee Break**		**Coffee Break**	**Coffee Break**	
	Chair: Dirk Nuyens	Chair: Jan Hesthaven			Chair: Hermann Matthies	
4:00-4:30 p.m.	Mikhail Tretyakov	Zouheir Rezki		Bus to KAUST	Eric Hall	
4:30-5:00 p.m.	Robert Patterson	Mohamed El Beltagy		Advisory Board Meeting	Bus to KAUST	
5:00-5:30 p.m.	Juho Häppölä	Performance at Library: David Keyes	Advisory Board Meeting			
5:30-6:00 p.m.	Poster Setup	Poster Session: KAUST University Library		Poster Session & Cultural Activity at Bay La Sun		Private discussions
6:00-6:30 p.m.	Welcome Reception: University Library					Poster Session & Cultural Activity at Bay La Sun. Closing remarks and Farewell
6:30 -7:30 p.m.		Conference Dinner: Al-Marsa Restaurant & Music By invitation only		Banquet Economic City By invitation only		
7:30 -8:30 p.m.						
8:30-9:15 p.m.				Bus to KAUST		

Contents

Oral presentations

Poster session I Sampling methods

Poster session II Bayesian Inference and Filtering

Poster session III Stochastic Differential Equations

Poster session IV Green Wireless Communication

Poster session VII Other Applications

Oral presentations

Application of quasi-Monte Carlo methods to PDEs with random coefficients – a survey of analysis and implementation

Frances Kuo, Josef Dick, Thong Le Gia, James Nichols, Ian Sloan, Ivan Graham, Robert Scheichl, Dirk Nuyens and Christoph Schwab.*

In this talk I will provide a survey of recent research efforts on the application of quasi-Monte Carlo (QMC) methods to PDEs with random coefficients. Such PDE problems occur in the area of uncertainty quantification. In recent years many papers have been written on this topic using a variety of methods. QMC methods are relatively new to this application area. I will consider different models for the randomness (uniform versus lognormal) and contrast different QMC algorithms (single-level versus multi-level, first order versus higher order, deterministic versus randomized). I will give a summary of the QMC error analysis and proof techniques in a unified view, and provide a practical guide to the software for constructing QMC points tailored to the PDE problems.

Frances Kuo
School of Mathematics and Statistics University of New South Wales Sydney NSW 2052 Australia
e-mail: f.kuo@unsw.edu.au

Bayesian inversion on an insulin-glucose system

Dirk Nuyens, Pieter Gillard and Piers Lawrence*

Bayesian inversion techniques to identify parameters of a mathematical model have started to make use of high-dimensional integration methods in recent years, see Stewart (2010) and Schillings & Schwab (2013). This in contrast with the traditional use of Markov chain Monte Carlo algorithms which are limited to Monte Carlo rates of convergence. We start from a real life problem and use a mathematical model for the insulin-glucose system in the human body, with the aim of identifying parameters for type-I diabetes patients. These parameters can then be used to adjust insulin therapy of the patient. This setting quickly delivers us hundreds of dimensions without even considering Banach space valued parameters. Our method of choice for the high dimensional integrals which appear are quasi-Monte Carlo methods.

Dirk Nuyens*, Pieter Gillard and Piers Lawrence
Numerical Analysis and Applied Mathematics Section, KU Leuven
e-mail: dirk.nuyens@cs.kuleuven.be

Chemical model reduction under uncertainty

Habib Najm, R. Malpica Galassi, M. Valorani*

We outline a strategy for chemical kinetic model reduction under uncertainty. We present highlights of our existing deterministic model reduction strategy, and describe the extension of the formulation to include parametric uncertainty in the detailed mechanism. We discuss the utility of this construction, as applied to hydrocarbon fuel-air kinetics, and the associated use of uncertainty-aware measures of error between predictions from detailed and simplified models.

Habib Najm
Sandia National Laboratories California
e-mail: hnnajm@sandia.gov

Quasi optimal and adaptive sparse grids with control variates for PDEs with random diffusion coefficient

Lorenzo Tamellini

In this talk we discuss possible strategies to minimize the impact of the *curse of dimensionality* effect when building sparse-grid approximations of a multivariate function $u = u(y_1, ..., y_N)$. More precisely, we present a "knapsack approach", in which we estimate the cost and the "error reduction" contribution of each possible component of the sparse grid, and then we choose the components with the highest "error reduction"/cost ratio. The estimates of the "error reduction" are obtained by either a mixed "a-priori"/"a-posteriori" approach, in which we first derive a theoretical bound and then tune it with some inexpensive auxiliary computations (resulting in the so-called "quasi-optimal sparse grids"), or by a "fully a-posteriori" approach (obtaining the so-called "adaptive sparse grids"). This framework is very general and can be used to build quasi-optimal/adaptive sparse grids on bounded and unbounded domains (e.g. u depending on uniform and normal random distributions for y_n), using both nested and non-nested families of univariate collocation points. We present some theoretical convergence results as well as numerical results showing the efficiency of the proposed approach for the approximation of the solution of elliptic PDEs with random diffusion coefficients. In this context, to treat the case of rough permeability fields in which a sparse grid approach may not be suitable, we propose to use the sparse grids as a control variate in a Monte Carlo simulation.

References:

1. Nobile, F., Tamellini, L., Tempone, R.: Comparison of Clenshaw–Curtis and Leja quasi-optimal sparse grids for the approximation of random PDEs. In: Spectral and High Order Methods for Partial Differential Equations - ICOSAHOM '14, *Lecture Notes in Computational Science and Engineering*, vol. 106, Springer (2015).
2. Nobile, F., Tamellini, L., Tempone, R.: Convergence of quasi-optimal sparse-grid approximation of Hilbert-space-valued functions: application to random elliptic PDEs. Accepted for publication on Numerische Mathematik, doi:10.1007/s00211-015-0773-y
3. Beck, J., Nobile, F., Tamellini, L., Tempone, R.: A Quasi-optimal Sparse Grids Procedure for Groundwater Flows. In: Spectral and High Order Methods for Partial Differential Equations - ICOSAHOM 2012, *Lecture Notes in Computational Science and Engineering*, vol. 95, pp. 1–16. Springer (2014).
4. Beck, J., Nobile, F., Tamellini, L., Tempone, R.: On the optimal polynomial approximation of stochastic PDEs by Galerkin and collocation methods. Mathematical Models and Methods in Applied Sciences **22**(09) (2012).

Lorenzo Tamellini
Dipartimento di Matematica "F. Casorati", Universitá di Pavia, Italy,
e-mail: lorenzo.tamellini@unipv.it

Recursive k-d Darts sampling for exploring high-dimensional spaces

Mohamed Ebeida, Ahmad Rushdi, Laura Swiler, Scott Mitchell, John Owens, Saman Ashkiani, Anjul Patney.*

We introduce Recursive k-d Darts: a new hyperplane sampling algorithm to estimate statistical metrics (e.g., mean and tail-probability) of an underlying black-box high-dimensional function. Our method decomposes the high-dimensional problem into a set of 1-dimensional problems. This approach enables efficient handling of discontinuities and higher-order estimates in smooth regions. We quantify estimation errors by comparing a local and global surrogate models, built on the fly as sampling proceeds, and use that to guide future samples.

Mohamed Ebeida
Sandia National Laboratories
e-mail: msebeid@sandia.gov

Multilevel sequential Monte-Carlo samplers

Ajay Jasra

Multilevel Monte-Carlo methods provide a powerful computational technique for reducing the computational cost of estimating expectations for a given computational effort. They are particularly relevant for computational problems when approximate distributions are determined via a resolution parameter h, with h=0 giving the theoretical exact distribution (e.g. SDEs or inverse problems with PDEs). The method provides a benefit by coupling samples from successive resolutions, and estimating differences of successive expectations. We develop a methodology that brings Sequential Monte-Carlo (SMC) algorithms within the framework of the Multilevel idea, as SMC provides a natural set-up for coupling samples over different resolutions. We prove that the new algorithm indeed preserves the benefits of the multilevel principle, even if samples at all resolutions are now correlated.

Ajay Jasra
Department of Statistics and Applied Probability (DSAP), National University of Singapore.
e-mail: staja@nus.edu.sg

Simultaneous reconstruction of outer boundary shape and conductivity distribution in electrical impedance tomography

Nuutti Hyvönen

The simultaneous retrieval of the exterior boundary shape and the interior admittivity distribution of an examined body in electrical impedance tomography is considered. The reconstruction method is built for the complete electrode model and it is based on the Frechet derivative of the corresponding current-to-voltage map with respect to the body shape. The reconstruction problem is cast into the Bayesian framework, and maximum a posteriori estimates for the admittivity and the boundary geometry are computed. The feasibility of the approach is evaluated by experimental data from water tank measurements.

Nuutti Hyvönen
Aalto University, Finland,
e-mail: nuutti.hyvonen@aalto.fi

Bayesian optimal experimental design for priors of compact support

Quan Long

In this study, we optimize the experimental setup computationally by optimal experimental design (OED) in a Bayesian framework. We approximate the posterior probability density functions (pdf) using truncated Gaussian distributions in order to account for the bounded domain of the uniform prior pdf of the parameters. The underlying Gaussian distribution is obtained in the spirit of the Laplace method, more precisely, the mode is chosen as the maximum a posteriori (MAP) estimate, and the covariance is chosen as the negative inverse of the Hessian of the misfit function at the MAP estimate. The model related entities are obtained from a polynomial surrogate. The optimality, quantified by the information gain measures, can be estimated efficiently by a rejection sampling algorithm against the underlying Gaussian probability distribution, rather than against the true posterior. This approach offers a significant error reduction when the magnitude of the invariants of the posterior covariance are comparable to the size of the bounded domain of the prior. We demonstrate the accuracy and superior computational efficiency of our method for shock-tube experiments aiming to measure the model parameters of a key reaction which is part of the complex kinetic network describing the hydrocarbon oxidation. In the experiments, the initial temperature and fuel concentration are optimized with respect to the expected information gain in the estimation of the parameters of the target reaction rate. We show that the expected information gain surface can change its "shape" dramatically according to the level of noise introduced into the synthetic data. The information that can be extracted from the data saturates as a logarithmic function of the number of experiments, and few experiments are needed when they are conducted at the optimal experimental design conditions.

Quan Long
United Technologies Research Center
e-mail: Quan.Long@kaust.edu.sa

Bayesian techniques for fatigue life prediction and for inference in linear time dependent PDEs

Marco Scavino

In this talk we introduce first the main characteristics of a systematic statistical approach to model calibration, model selection and model ranking when stress-life data are drawn from a collection of records of fatigue experiments. Focusing on Bayesian prediction assessment, we consider fatigue-limit models and random fatigue-limit models under different a priori assumptions. In the second part of the talk, we present a hierarchical Bayesian technique for the inference of the coefficients of time dependent linear PDEs, under the assumption that noisy measurements are available in both the interior of a domain of interest and from boundary conditions. We present a computational technique based on the marginalization of the contribution of the boundary parameters and apply it to inverse heat conduction problems.

References:

1. "Bayesian inference and model comparison for metallic fatigue data", joint work with Ivo Babüska, Zaid Sawlan, Barna Szab and Raúl Tempone, submitted, arXiv:1512.01779
2. "A hierarchical Bayesian setting for an inverse problem in linear parabolic PDEs with noisy boundary conditions", joint work with Fabrizio Ruggeri, Zaid Sawlan and Raúl Tempone, submitted, arXiv:1501.04739

Marco Scavino
Computer, Electrical and Mathematical Sciences & Engineering Division King Abdullah University of Science and Technology (KAUST), Saudi Arabia.
e-mail: marco.scavino@kaust.edu.sa

Geometric integrators for stochastic rigid body dynamics

Mikhail Tretyakov

Geometric integrators play an important role in simulating dynamical systems on long time intervals with high accuracy. We will illustrate geometric integration ideas within the stochastic context, mostly on examples of stochastic thermostats for rigid body dynamics. The talk will be mainly based on joint recent work with Rusland Davidchak and Tom Ouldridge.

Mikhail Tretyakov
School of Mathematical Sciences, The University of Nottingham University Park Nottingham, NG7 2RD
e-mail: Michael.Tretyakov@nottingham.ac.uk

Simulations of flame generated particles

Robert Patterson

The nonlinear structure of the equations describing the evolution of a population of coagulating particles in a flame make the use of stochastic particle methods attractive for numerical purposes. I will present an analysis of the stochastic fluctuations inherent in these numerical methods leading to an efficient sampling technique for steady-state problems. I will also give some examples where stochastic particle methods have been used to explore the effect of uncertain parameters in soot formation models. In conclusion I will try to indicate some of the issues in optimising these methods for the study of uncertain model parameters.

Robert Patterson
Weierstrass Institute for Applied Analysis and Stochastics, Berlin
e-mail: Robert.Patterson@wias-berlin.de

Error analysis in Fourier methods for option pricing

Juho Häppölö

We provide a bound for the error committed when using a Fourier method to price European options when the underlying follows an exponential Levy dynamic. The price of the option is described by a partial integro-differential equation (PIDE). Applying a Fourier transformation to the PIDE yields an ordinary differential equation that can be solved analytically in terms of the characteristic exponent of the Levy process. Then, a numerical inverse Fourier transform allows us to obtain the option price. We present a novel bound for the error and use this bound to set the parameters for the numerical method. We analyze the properties of the bound for a dissipative and pure-jump example. The bound presented is independent of the asymptotic behaviour of option prices at extreme asset prices. The error bound can be decomposed into a product of terms resulting from the dynamics and the option payoff, respectively. The analysis is supplemented by numerical examples that demonstrate results comparable to and superior to the existing literature.

Juho Häppölö
Computer, Electrical and Mathematical Sciences & Engineering Division King Abdullah University of Science and Technology (KAUST), Saudi Arabia
e-mail: juho.happola@kaust.edu.sa

Surrogate based approaches to parameter inference in ocean models

Omar Knio

This talk discusses the inference of physical parameters using model surrogates. Attention is focused on the use of sampling schemes to build suitable representations of the dependence of the model response on uncertain input data. Non-intrusive spectral projections and regularized regressions are used for this purpose. A Bayesian inference formalism is then applied to update the uncertain inputs based on available measurements or observations. To perform the update, we consider two alternative approaches, based on the application of Markov Chain Monte Carlo methods or of adjoint-based optimization techniques. We outline the implementation of these techniques to infer dependence of wind drag, bottom drag, and internal mixing coefficients.

Omar Knio
Computer, Electrical and Mathematical Sciences & Engineering Division King Abdullah University of Science and Technology (KAUST), Saudi Arabia
e-mail: omar.knio@kaust.edu.sa

Emulation of numerical models with over-specified basis functions

Bani Mallick

We propose a Bayesian approach to statistical inference in emulation and calibration of a numerical model with a basis-function representation. Numerical models are commonly used now-a-days as a surrogate for real-life events or experiments which, due to either rarity of occurrence or associated expenses, can be observed only a limited number of occurrences of this event. The goal of our modeling effort is to match the numerical model output with the ones collected from actual events. In addition to unknown parameters in the field experiments, the input-output relationship is also treated as unknowns, allowing a full treatment of all possible sources of uncertainty. To combine these field observations with a collection of runs from the numerical model, we employ a fully model-based approach using the Kennedy-O'Hagan framework of computer model validation. Compared to the conventional Gaussian process emulators, we have achieved greater efficiency with a basis-function representation in terms of smaller predictive uncertainty, greater control over model sparsity and shorter computational time. We have developed an efficient estimation scheme that allows the user to treat the number of functions and their inclusion probabilities as unknown quantities and to estimate them via a reversible jump Monte Carlo sampler. Here, we use a generalized polynomial chaos expansion - depending on the stochastic model for the input, an optimal class of orthonormal polynomial functionals is chosen from the Askey scheme to represent the emulator. We show that this hierarchical specification provides prior support for a large family of response functions. Along with several simulation examples focusing on different model characteristics, our approach is also implemented with a real dataset from a series of laboratory experiments related to astrophysics.

Bani Mallick
Texas A&M University
e-mail: bmallick@stat.tamu.edu

A sparse stochastic collocation technique for high frequency wave propagation with uncertainty

Olof Runborg

We consider the wave equation with highly oscillatory initial data, where there is uncertainty in the wave speed, initial phase and/or initial amplitude. To estimate quantities of interest related to the solution and their statistics, we combine a high-frequency method based on Gaussian beams with sparse stochastic collocation. Although the wave solution, u^ε, is highly oscillatory in both physical and stochastic spaces, we provide theoretical arguments and numerical evidence that quantities of interest based on local averages of $|u^\varepsilon|^2$ are smooth, with derivatives in the stochastic space uniformly bounded in ε, where ε denotes the short wavelength. This observable related regularity makes the sparse stochastic collocation approach more efficient than Monte Carlo methods. We present numerical tests that demonstrate this advantage.

Olof Runborg
Royal Institute of Technology (KTH), Sweden
e-mail: olofr@nada.kth.se

Uncertainty quantification for subsurface flow problems

Claudia Schillings

The Ensemble Kalman filter (EnKF) has had enormous impact on the applied sciences since its introduction in the 1990s by Evensen and coworkers. In this talk, we will discuss an analysis of the EnKF based on the continuous time scaling limits, which allows to study the properties of the EnKF for fixed ensemble size. The theoretical considerations give useful insights into properties of the method and provide tools for a systematic development and improvement. Results from various numerical experiments supporting the theoretical findings will be presented. This is joint work with Andrew M. Stuart (University of Warwick) and part of the EPSRC-funded project EQUIP.

Claudia Schillings
Mathematics Institute, University of Warwick
e-mail: c.schillings@warwick.ac.uk

A new smoothing technique for basket options

Markus Siebenmorgen, Christian Bayer and Raúl Tempone*

The computation of the price of European basket options in a Black-Scholes model leads in certain cases to the calculation of the integral

$$E\left[\left(\sum_{i=1}^{d} w_i e^{X_i} - K\right)^+\right], \tag{1}$$

where X follows $\mathcal{N}(0, \Sigma)$ with a covariance matrix Σ and $d >> 1$. Hence, we have to compute an integral over the integration domain $\mathbb{R}^d$ for an integrand with a kink. We provide a simple smoothing method which produces an analytic integrand and is able to reduce the dimensionality of the integration problem by 1. Moreover, this smoothing does not introduce any approximation error. In particular, we transform the d-dimensional random variable in such a way that it is feasible to apply the famous Black-Scholes formula with respect to a single coordinate. The resulting integration problem over $\mathbb{R}^{d-1}$ of an analytic function is then solved by an adaptive sparse grid approach. This leads, at least in considerably high dimensions, to better convergence results compared to those of standard Monte Carlo or quasi-Monte Carlo quadratures.

Markus Siebenmorgen
Institute for Numerical Simulation, University of Bonn, Germany
e-mail: siebenmorgen@ins.uni-bonn.de

Approximation of quantum observables by molecular dynamics simulations

Mattias Sandberg

In this talk I will discuss how to estimate the uncertainty in molecular dynamics simulations. Molecular dynamics is a computational method to study molecular systems in materials science, chemistry, and molecular biology. The wide popularity of molecular dynamics simulations relies on the fact that in many cases it agrees very well with experiments. If we however want the simulation to predict something that has no comparing experiment, we need a mathematical estimate of the accuracy of the computation. In the case of molecular systems with few particles, such studies are made by directly solving the Schrödinger equation. In this talk I will discuss theoretical results on the accuracy between quantum mechanics and molecular dynamics, to be used for systems that are too large to be handled computationally by the Schrödinger equation.?

Mattias Sandberg
Royal Institute of Technology (KTH), Sweden
e-mail: msandb@kth.se

A Filtering Approach for Bayesian Inversion

Hermann Matthies

The inverse problem of determining data (coefficient fields) in an SPDE model from observations (or some other computational model) is a computationally intensive task, and is intimately tied to being able to compute a conditional expectation. The talk will quickly review the Bayesian setting in connection with the conditional expectation, and then concentrate on the filter-like algorithms and look at the various approximations involved. The conditional expectation in its original concept is just an orthogonal projection, but when factored through a possibly non-linear observation operator, it becomes more complicated, and can typically not be computed exactly. This involves further approximation, involving finite dimensional subspaces onto which to approximate the conditional expectation. The next question to address is which characteristics of the posterior to compute and update. The filter algorithms typically correct for the conditional mean, leaving anything else unchanged. This gives a mapping from prior to posterior variable. Further characteristics become more involved, and transport mappings seem a possibility for more accurate filters.

Hermann Matthies
Institute of Scientific Computing, Technical University of Braunschweig
e-mail: wire@tu-braunschweig.de

The multilevel particle filter

Kody Law

This talk will pertain to the filtering of partially observed diffusions, with discrete-time observations. It is assumed that only biased approximations of the diffusion can be obtained, for choice of an accuracy parameter indexed by ℓ. A multilevel estimator is proposed, consisting of a telescopic sum of increment estimators associated to the successive levels. The work associated to $\mathcal{O}(\varepsilon^2)$ mean-square error between the multilevel estimator and average with respect to the filtering distribution is shown to scale optimally, for example as $\mathcal{O}(\varepsilon^2)$ for optimal rates of convergence of the underlying diffusion approximation. The method is illustrated on some toy examples as well as estimation of interest rate based on real S&P 500 stock price data.

Kody Law
Oak Ridge National Laboratory
e-mail: lawkj@ornl.gov, kodylaw@gmail.com

The race for 5G wireless networks

Khaled Ben Letaief

The need for the next-generation of wireless networks, commonly referred to as 5G networks is being driven by the ever-increasing demands for mobile data and the emergence of new applications such as IoT or the Internet of Things and the Tactile Internet. In this talk, we will discuss the future trends in wireless communications and identify the key air interface and network architecture technologies that are required to meet the stringent demands of 5G wireless networks. This talk will also introduce Hamad Bin Khalifa University, a newly established research-intensive University in Qatar

Khaled Ben Letaief
Department of Electronic and Computer Engineering, Purdue University, Indiana, USA
e-mail: eekhaled@ust.hk

Secure Communications over Wireless Networks Even 1 bit Feedback Helps Achieving Security

Zouheir Rezki

Recently, there have been a surge toward developing sophisticated security mechanisms based on a cross layer design. While an extensive progress has been realized toward establishing physical layer security as an important design paradigm to enhance security of existing wireless networks, only a little effort has been made toward designing practical coding schemes that achieve or approach the secrecy capacity. Most of existing results are tied to some simplifying assumptions that do not seem always reasonable (passive eavesdropper, perfect channel state information (CSI), etc.). Furthermore, it is still not very clear how to exploit physical layer security paradigms, together with existing cryptosystems, in order to add a supplementary level of protection for information transmission or to achieve key agreement. In this talk, we address the first part of the above problematic, i.e., the effect of channel uncertainty on network security. Particularly, we show that even a coarse estimate of the main channel (channel between the transmitter and the legitimate receiver) can help providing a positive secrecy rate. Specifically, we assume two types of channel uncertainty at the transmitter. The first one is a rate-limited feedback in a block fading channel where the feedback information can be proactive (at the beginning of the coherence block) or of ARQ-type. The second type of uncertainty takes the form of a noisy estimate of the main channel at the transmitter in a fast fading channel. In both cases, we provide upper and lower bounds on the secrecy capacity. We argue how our achievable schemes and upper bounding techniques extend to multi-user setting (broadcasting a single confidential message or multiple confidential messages to multiple legitimate receivers) and to multiple antenna channels.

Zouheir Rezki
Computer, Electrical and Mathematical Sciences & Engineering Division King Abdullah University of Science and Technology (KAUST), Saudi Arabia
e-mail: Zouheir.rezki@kaust.edu.sa

Solution of stochastic nonlinear PDEs using Wiener-Hermite expansion of high orders

Mohamed El Beltagy

In this work, the Wiener-Hermite Expansion (WHE) is used to solve stochastic nonlinear PDEs excited with noise. The generation of the equivalent set of deterministic integro-differential equations is automated and hence allows for high order terms of WHE. The automation difficulties are discussed, solved and implemented to output the final system to be solved. A numerical Pikard-like algorithm is suggested to solve the resulting deterministic system. The automated WHE is applied to the 1D diffusion equation and to the heat equation. The results are compared with previous solutions obtained with WHEP (WHE with perturbation) technique. The solution obtained using the suggested WHE technique is shown to be the limit of the WHEP solutions with infinite number of corrections. The automation is extended easily to account for white-noise of higher dimension and for general nonlinear PDEs.

Mohamed El Beltagy
ECE Department, Engineering College, Effat University, Jeddah, Saudi Arabia
e-mail: melbeltagy@effatuniversity.edu.sa

Energy landscape and the two-scale large deviations for biological stochastic dynamics

Tiejun Li, Fangting Li, Xianggang Li and Cheng Lv*

The construction of energy landscape for bio-dynamics is attracting more and more attention recent years. In this talk, I will introduce the strategy to construct the landscape from the connection to rare events, which relies on the large deviation theory for Gillespie-type jump dynamics. In the application to a typical genetic switching model, the two-scale large deviation theory is developed to take into account the fast switching of DNA states. The comparison with other proposals are also discussed. We demonstrate different diffusive limits arise when considering different regimes for genetic translation and switching processes.

Tiejun Li
School of Mathematical Sciences, Peking University, No. 5 Yiheyuan Road, Haidian District, Beijing, 100871
e-mail: tieli@math.pku.edu.cn

Scalable algorithms for optimal control of stochastic PDEs

Omar Ghattas, Alen Alexanderian , Noemi Petra and Georg Stadler*

We present methods for the optimal control of systems governed by partial differential equations with infinite-dimensional uncertain parameters. We consider an objective function that involves the mean and variance of the control objective, leading to a risk-averse optimal control formulation. To make the optimal control problem computationally tractable, we employ a local quadratic approximation of the objective with respect to the uncertain parameter. This enables computation of the mean and variance of the control objective analytically. The resulting risk-averse optimization problem is formulated as a PDE-constrained optimization problem with constraints given by the forward and adjoint PDEs for the first and second-order derivatives of the quantity of interest with respect to the uncertain parameter, and with an objective that involves the trace of a covariance-preconditioned Hessian (of the objective with respect to the uncertain parameters) operator. A randomized trace estimator is used to make tractable the trace computation. Adjoint-based techniques are used to derive an expression for the infinite-dimensional gradient of the risk-averse objective function via the Lagrangian, leading to a quasi-Newton method for solution of the optimal control problem. A specific problem of optimal control of a linear elliptic PDE that describes flow of a fluid in a porous medium with uncertain permeability field is considered. We present numerical results to study the consequences of the local quadratic approximation and the efficiency of the method.

Omar Ghattas
University of Texas at Austin

Alen Alexanderian
NCSU

Noemi Petra at UC Merced · Georg Stadler at NYU
e-mail: omar@ices.utexas.edu

Hierarchical low-rank approximation for high dimensional approximation

Anthony Nouy

Tensor methods are among the most prominent tools for the numerical solution of high-dimensional problems where functions of multiple variables have to be approximated. Such high-dimensional approximation problems naturally arise in stochastic analysis and uncertainty quantification. In many practical situations, the approximation of high-dimensional functions is made computationally tractable by using rank-structured approximations. In this talk, we present algorithms for the approximation in hierarchical tensor format using statistical methods. Sparse representations in a given tensor format are obtained with adaptive or convex relaxation methods, with a selection of parameters using cross-validation methods.

Anthony Nouy
Ecole Centrale de Nantes, GeM UMR 6183, Nantes, France
e-mail: anthony.nouy@ec-nantes.fr

Estimation of parameter sensitivities for stochastic reaction networks

Ankit Gupta

Quantification of the effects of parameter uncertainty is an important and challenging problem in Systems Biology. We consider this problem in the context of stochastic models of biochemical reaction networks where the dynamics is described as a continuous-time Markov chain whose states represent the molecular counts of various species. For such models, effects of parameter uncertainty are often quantified by estimating the infinitesimal sensitivities of some observables with respect to model parameters. The aim of this talk is to present a holistic approach towards this problem of estimating parameter sensitivities for stochastic reaction networks. Our approach is based on a generic formula which allows us to construct efficient estimators for parameter sensitivity using simulations of the underlying model. We will discuss how novel simulation techniques, such as tau-leaping approximations, multi-level methods etc. can be easily integrated with our approach and how one can deal with "stiff" reaction networks where reactions span multiple time-scales. We will demonstrate the efficiency and applicability of our approach using many examples from the biological literature.

Ankit Gupta
Department of Biosystems Science and Engineering, ETH Zurich, Switzerland
e-mail: ankit.gupta@bsse.ethz.ch

An efficient forward-reverse expectation-maximization algorithm for statistical inference in stochastic reaction networks.

Pedro Vilanova

In this work, we present an extension of the forward-reverse representation introduced in "Simulation of forward-reverse stochastic representations for conditional diffusions", a 2014 paper by Bayer and Schoenmakers to the context of stochastic reaction networks (SRNs). We apply this stochastic representation to the computation of efficient approximations of expected values of functionals of SRN bridges, i.e., SRNs conditional on their values in the extremes of given time-intervals. We then employ this SRN bridge-generation technique to the statistical inference problem of approximating reaction propensities based on discretely observed data. To this end, we introduce a two-phase iterative inference method in which, during phase I, we solve a set of deterministic optimization problems where the SRNs are replaced by their reaction-rate ordinary differential equations approximation; then, during phase II, we apply the Monte Carlo version of the Expectation-Maximization algorithm to the phase I output. By selecting a set of over-dispersed seeds as initial points in phase I, the output of parallel runs from our two-phase method is a cluster of approximate maximum likelihood estimates. Our results are supported by numerical examples.

Pedro Vilanova
Computer, Electrical and Mathematical Sciences & Engineering Division King Abdullah University of Science and Technology (KAUST), Saudi Arabia
e-mail: pedro.vilanova@kaust.edu.sa

Static models, recursive estimators and the zero-variance approach

Gerardo Rubino

When evaluating dependability aspects of complex systems, most models belong to the static world, where time is not an explicit variable. These models suffer from the same problems than dynamic ones (stochastic processes), such as the frequent combinatorial explosion of the state spaces. In the Monte Carlo domain, on of the most significant difficulties is the rare event situation. In this talk, we describe this context and a recent technique that appears to be at the top performance level in the area, where we combined ideas that lead to very fast estimation procedures with another approach called zero-variance approximation. Both ideas produced a very efficient method that has the right theoretical property concerning robustness, the Bounded Relative Error one. Some examples illustrate the results.

Gerardo Rubino
IRISA/INRIA Campus de Beaulieu, 35042 RENNES Cedex
e-mail: Gerardo.Rubino@inria.fr

A potpourri of results from the KAUST SRI-UQ

Raúl Tempone

As the KAUST Strategic Research Initiative for Uncertainty Quantification completes its fourth year of existence we recall several results produced during its exciting journey of discovery. These include, among others, contributions on Multi-level and Multi-index sampling techniques that address both direct and inverse problems. We may discuss also several techniques for Bayesian Inverse Problems and Optimal Experimental Design.

Raúl Tempone
Computer, Electrical and Mathematical Sciences & Engineering Division King Abdullah University of Science and Technology (KAUST), Saudi Arabia
e-mail: raul.tempone@kaust.edu.sa

Gaussian process emulators in Bayesian inverse problems

Aretha Teckentrup

A major challenge in the application of sampling methods to large scale inverse problems, is the high computational cost associated with solving the forward model for a given set of input parameters. To overcome this difficulty, we consider using a surrogate model that approximates the solution of the forward model at a much lower computational cost. We focus in particular on Gaussian process emulators, and analyse the error in the posterior distribution resulting from this approximation.

Aretha Teckentrup
Mathematics Institute, University of Warwick
e-mail: a.teckentrup@warwick.ac.uk

Optimal mesh hierarchies in Multilevel Monte Carlo methods

Erik von Schwerin

I will discuss how to choose optimal mesh hierarchies in Multilevel Monte Carlo (MLMC) simulations when computing the expected value of a quantity of interest depending on the solution of, for example, an Ito stochastic differential equation or a partial differential equation with stochastic data. I will consider numerical schemes based on uniform discretization methods with general approximation orders and computational costs. I will compare optimized geometric and non-geometric hierarchies and discuss how enforcing some domain constraints on parameters of MLMC hierarchies affects the optimality of these hierarchies. I will also discuss the optimal tolerance splitting between the bias and the statistical error contributions and its asymptotic behavior. This talk presents joint work with N.Collier, A.-L.Haji-Ali, F. Nobile, and R. Tempone.

Erik von Schwerin
Department of Mathematical Sciences, University of Delaware
e-mail: schwerin@udel.edu, erik.von.schwerin@gmail.com

Multilevel ensemble Kalman filtering

Håkon Hoel, Alexey Chernov, Kody J. H. Law, Fabio Nobile, and Raúl Tempone*

The ensemble Kalman filter (EnKF) is a sequential filtering method that uses an ensemble of particle paths to estimate the means and covariances required by the Kalman filter by the use of sample moments, i.e., the Monte Carlo method. EnKF is often both robust and efficient, but its performance may suffer in settings where the computational cost of accurate simulations of particles is high. The multilevel Monte Carlo method (MLMC) is an extension of classical Monte Carlo methods which by sampling stochastic realizations on a hierarchy of resolutions may reduce the computational cost of moment approximations by orders of magnitude. In this work we have combined the ideas of MLMC and EnKF to construct the multilevel ensemble Kalman filter (MLEnKF) for the setting of finite dimensional state and observation spaces. The main ideas of this method is to compute particle paths on a hierarchy of resolutions and to apply multilevel estimators on the ensemble hierarchy of particles to compute Kalman filter means and covariances. Theoretical results and a numerical study of the performance gains of MLEnKF over EnKF will be presented. Some ideas on the extension of MLEnKF to settings with infinite dimensional state spaces will also be presented.

Håkon Hoel
Department of Mathematics, University of Oslo, Norway
e-mail: haakonah@math.uio.no, haakonah1@gmail.com

Adaptive stochastic Galerkin FEM with hierarchical tensor representations

Martin Eigel

PDE with stochastic data usually lead to very high-dimensional algebraic problems which easily become unfeasible for numerical computations because of the dense coupling structure of the discretised stochastic operator. Recently, an adaptive stochastic Galerkin FEM based on a residual a posteriori error estimator was presented and the convergence of the adaptive algorithm was shown. While this approach leads to a drastic reduction of the complexity of the problem due to the iterative discovery of the sparsity of the solution, the problem size and structure is still rather limited. To allow for larger and more general problems, we exploit the tensor structure of the parametric problem by representing operator and solution iterates in the tensor train (TT) format. The (successive) compression carried out with these representations can be seen as a generalisation of some other model reduction techniques, e.g. the reduced basis method. We show that this approach facilitates the efficient computation of different error indicators related to the computational mesh, the active polynomial chaos index set, and the TT rank. In particular, the curse of dimension is avoided.

Martin Eigel
Weierstrass Institute, Berlin, Germany
e-mail: eigel@wias-berlin.de

A study of Monte Carlo methods for weak approximations of stochastic particle systems in the mean-field

Abdul Lateef Haji Ali

I discuss using single level and multilevel Monte Carlo methods to compute quantities of interests of a stochastic particle system in the mean-field. In this context, the stochastic particles follow a coupled system of Ito stochastic differential equations (SDEs). Moreover, this stochastic particle system converges to a stochastic mean-field limit as the number of particles tends to infinity. I start by recalling the results of applying different versions of Multilevel Monte Carlo (MLMC) for particle systems, both with respect to time steps and the number of particles and using a partitioning estimator. Next, I expand on these results by proposing the use of our recent Multi-index Monte Carlo method to obtain improved convergence rates.

Abdul Lateef Haji Ali
Computer, Electrical and Mathematical Sciences & Engineering Division King Abdullah University of Science and Technology (KAUST), Saudi Arabia
e-mail: abdullateef.hajiali@kaust.edu.sa

Computable error estimates for Monte Carlo finite element approximation of elliptic PDE with lognormal diffusion coefficients

Eric Hall, Håkon Hoel, Mattias Sandberg, Anders Szepessy and Raúl Tempone.*

The Monte Carlo (and Multi-level Monte Carlo) finite element method can be used to approximate observables of solutions to diffusion equations with lognormal distributed diffusion coefficients, e.g. modeling ground water flow. Typical models use lognormal diffusion coefficients with Hölder regularity of order up to 1/2 a.s. This low regularity implies that the high frequency finite element approximation error (i.e. the error from frequencies larger than the mesh frequency) is not negligible and can be larger than the computable low frequency error. We address how the total error can be estimated by the computable error.

Eric Hall
Department of Mathematics and Statistics, Lederle Graduate Research Tower, University of Massachusetts
e-mail: hall@math.umass.edu

VPS: Voronoi Piecewise Surrogate models for high-dimensional data fitting

Ahmad Rushdi

We introduce a new method to construct credible global surrogate models with local accuracy in high-dimensional spaces: Voronoi Piecewise Surrogate (VPS) models. The key component in our method is to decompose the high-dimensional parameter space using an implicit Voronoi tessellation around the known function evaluations as seeds. VPS assigns samples to cells using a simple nearest seed search, and finds cell neighbors via local hyperplane sampling, without constructing an explicit mesh. To avoid the intractable complexity of high-d Voronoi cells, we construct an approximate dual Delaunay graph to establish the neighborhood network between cells. Each cell then uses information at its neighbors to build its own local piece of the global surrogate. This approach breaks down the high-order approximation problem into a set of piecewise low-order problems in the neighborhood of each function evaluation. The one-to-one mapping between the number of function evaluations and the number of Voronoi cells, regardless of the number of dimensions, eliminates the curse of dimensionality associated with standard domain decompositions. Furthermore, the Voronoi tessellation is naturally updated with the addition of new function evaluations. Due to its piecewise nature, VPS accurately handles smooth functions with high curvature as well as functions with discontinuities, and can be implemented in parallel.

University of Texas, Austin, USA
e-mail: arushdi@utexas.edu ; arushdi@sandia.gov

Multi-Index Monte Carlo and stochastic collocation methods for random PDEs.

Fabio Nobile, Abdul-Lateef Haji Ali, Lorenzo Tamellini and Raúl Tempone*

In this talk we consider the problem of computing statistics of the solution of a partial differential equation with random data, where the random coefficient is parametrized by means of a finite or countable sequence of terms in a suitable expansion. We describe and analyze a Multi-Index Monte Carlo (MIMC) and a Multi-Index Stochastic Collocation method (MISC). the former is both a stochastic version of the combination technique introduced by Zenger, Griebel and collaborators and an extension of the Multilevel Monte Carlo (MLMC) method first described by Heinrich and Giles. Instead of using first-order differences as in MLMC, MIMC uses mixed differences to reduce the variance of the hierarchical differences dramatically. This in turn yields new and improved complexity results, which are natural generalizations of Giles's MLMC analysis, and which increase the domain of problem parameters for which we achieve the optimal convergence, $\mathcal{O}(\mathrm{TOL}^{-2})$. On the same vein, MISC is a deterministic combination technique based on mixed differences of spatial approximations and quadratures over the space of random data. Provided enough mixed regularity, MISC can achieve better complexity than MIMC. Moreover, we show that in the optimal case the convergence rate of MISC is only dictated by the convergence of the deterministic solver applied to a one-dimensional spatial problem. We propose optimization procedures to select the most effective mixed differences to include in MIMC and MISC. Such optimization is a crucial step that allows us to make MIMC and MISC computationally effective. We finally show the effectiveness of MIMC and MISC with some computational tests, including tests with a infinite countable number of random parameters.

Fabio Nobile
Ecole Polytechnique Fdrale de Lausanne (EPFL), Lausanne, CH-1015, Switzerland
e-mail: fabio.nobile@epfl.ch

The Red Sea Ensemble Forecasting System: Assimilation, Visualization and Control under Uncertainties

Ibrahim Hoteit

The talk will present our ongoing efforts to build an efficient and fully parallel ensemble data assimilation system for forecasting the Red Sea circulation at high resolution. I will first describe this ensemble Kalman filter (EnKF)-based system and show some assimilation results and then discuss some of our recent contributions to enhance the efficiency and performances of EnKFs. The second part will present developments for efficiently visualizing and mining the outputted big data and for decision making and control under the estimated multiple ensemble scenarios and associated uncertainties.

Ibrahim Hoteit
Computer, Electrical and Mathematical Sciences & Engineering Division King Abdullah University of Science and Technology (KAUST), Saudi Arabia
e-mail: ibrahim.hoteit@kaust.edu.sa

On the predictive capabilities of multiphase Darcy flow models

Matteo Icardi and Serge Prudhomme*

Darcy's law is a widely used model and the limit of its validity is fairly well known. When the flow is sufficiently slow and the porosity relatively homogeneous and low, Darcy's law is the homogenized equation arising from the Stokes and Navier- Stokes equations and depends on a single effective parameter (the absolute permeability). However when the model is extended to multiphase flows, the assumptions are much more restrictive and less realistic. Therefore it is often used in conjunction with empirical models (such as relative permeability and capillary pressure curves), derived usually from phenomenological speculations and experimental data fitting. In this work, we present the results of a Bayesian calibration of a two-phase flow model, using high-fidelity DNS numerical simulation (at the pore-scale) in a realistic porous medium. These reference results have been obtained from a Navier-Stokes solver coupled with an explicit interphase-tracking scheme. The Bayesian inversion is performed on a simplified 1D model in Matlab by using adaptive spectral method. Several data sets are generated and considered to assess the validity of this 1D model.

Matteo Icardi
Mathematics Institute, University of Warwick
e-mail: matteo.icardi@warwick.ac.uk, mat.icardi@gmail.com

Polynomial Chaos Surrogates for Bayesian Inference

Olivier Le Maître

The Bayesian inference is a popular probabilistic method to solve inverse problems, such as the identification of field parameter in a PDE model. The inference rely on the Bayes rule to update the prior density of the sought field, from observations, and derive its posterior distribution. In most cases the posterior distribution has no explicit form and has to be sampled, for instance using a Markov-Chain Monte Carlo method. In practice the prior field parameter is decomposed and truncated (e.g. by means of Karhunen- Loéve decomposition) to recast the inference problem into the inference of a finite number of coordinates. Although proved effective in many situations, the Bayesian inference as sketched above faces several difficulties requiring improvements. First, sampling the posterior can be a extremely costly task as it requires multiple resolutions of the PDE model for different values of the field parameter. Second, when the observations are not very much informative, the inferred parameter field can highly depends on its prior which can be somehow arbitrary. These issues have motivated the introduction of reduced modeling or surrogates for the (approximate) determination of the parametrized PDE solution and hyper-parameters in the description of the prior field. Our contribution focuses on recent developments in these two directions: the acceleration of the posterior sampling by means of Polynomial Chaos expansions and the efficient treatment of parametrized covariance functions for the prior field. We also discuss the possibility of making such approach adaptive to further improve its efficiency.

Olivier Le Maître
Laboratoire d'Informatique pour la Mécanique et les Sciences de l'Ingénieur LIMSI-CNRS
e-mail: olm@limsi.fr

On goal-oriented formulations for reduced-order methods

Serge Prudhomme

In this talk, I will explore formulations by which one could obtain a reduced model, using e.g. low-rank approximation or so-called proper generalized decomposition methods, tailored to the calculation of quantities of interest. Such a paradigm represents a departure from classical approaches in which a general reduced model is first derived by minimization of the energy or of the residual and then adapted by controlling the error with respect to quantities of interest using dual-based error estimates. This presentation will be above all exploratory and will consist for the most part in a review of preliminary works available in the literature that address this problem.

Serge Prudhomme
Department of Mathematical and Industrial Engineering, École Polytechnique de Montréal, Canada
e-mail: serge.prudhomme@polymtl.ca

Estimation of uncertain parameters of large Matérn covariance functions with using hierarchical matrix technique

A. Litvinenko, M. Genton, Y. Sun, and D. Keyes

The class of Matérn covariance functions

$$C(\theta) = \frac{2\sigma^2}{\Gamma(\nu)} \left(\frac{r}{2l}\right)^{\nu} K_\nu \left(\frac{r}{l}\right), \quad \theta = (\sigma^2, \nu, l).$$

becomes very popular in spatial statistics and especially in geostatistics. In this work we use observations $\mathbf{z} = (z_1, ..., z_n)^T$ to estimate uncertain parameter(s) θ by maximizing the log-likelihood function

$$-2\mathcal{L}(\theta) = N\log 2\pi + \log\det\{C(\theta)\} + \mathbf{z}^T C(\theta)^{-1}\mathbf{z}.$$

On each iteration i of a maximization algorithm we have a new matrix $C(\theta_i)$. To speed up the computations, we approximate the likelihood $\mathcal{L}(\theta)$ by $\tilde{\mathcal{L}}(\theta, k)$, where k is the hierarchical matrix rank used for approximation of the covariance matrix $C(\theta) \approx C^{\mathcal{H}}(\theta, k)$.

We approximate large non-structured Matérn covariance matrices of size $n \times n$ in the hierarchical $(\mathcal{H})$-matrix format with a log-linear computational cost and storage $\mathcal{O}(kn\log n)$, where rank $k \ll n$ is a small integer. Further applications are: spatial statistics, machine learning, image analysis, kriging, Kalman filter update and optimal design. Such linear algebra operations as matrix setup, matrix-vector product, matrix-matrix product, matrix-inversion and matrix update have cost $\mathcal{O}(k^\alpha n\log^\alpha n)$, $\alpha = 1, 2$.

We demonstrate $\mathcal{H}$-matrix approximation of Matérn covariance functions for different smoothness parameters ν as well as for covariance lengths l. To characterize the approximation error we compute not only standard matrix norms, but also the Kulbnek-Leibner divergence.

References

1. B. N. Khoromskij, A. Litvinenko and H. G Matthies, *Application of hierarchical matrices for computing the Karhunen-Loéve expansion*, Computing, Vol. 84, Issue 1-2, pp 49-67, 2009, Springer Vienna.
2. B. N. Khoromskij and A. Litvinenko, *Data sparse computation of the karhunen-loève expansion*, AIP Conference Proceedings, 1048 (2008), p. 311.
3. A. Litvinenko and H. G. Matthies, *Sparse data representation of random fields*, PAMM, 9 (2009), pp. 587–588.
4. B. Matérn, *Spatial variation. Lecture notes in statistics.*, vol. 36, Springer-Verlag, 1986.
5. W. Nowak and A. Litvinenko, *Kriging and spatial design accelerated by orders of magnitude: combining low-rank covariance approximations with fft-techniques*, Mathematical Geosciences, 45 (2013), pp. 411–435.
6. W. Hackbusch, *Hierarchische Matrizen - Algorithmen und Analysis. Lecture notes.*, Max-Planck-Institut für Mathematik, Leipzig, 2004.
7. Y. Sun, M. Stein, *Statistically and computationally efficient estimating equations for large spatial datasets*, JCGS, 2015, to appear.
8. J. Castrillon-Candas, M. Genton, and R. Yokota, *Multi-Level Restricted Maximum Likelihood Covariance Estimation and Kriging for Large Non-Gridded Spatial Datasets*, arXiv:1504.00302v1, 2015.

A. Litvinenko, M. Genton, Y. Sun, and D. Keyes
Division of Computer, Electrical, and Mathematical Science and Engineering, King Abdullah University of Science and Technology, Thuwal, Saudi Arabia.
e-mail: alexander.litvinenko@kaust.edu.sa

Analysis of the stability and accuracy of the discrete least-squares approximation on multivariate polynomial spaces

Giovanni Migliorati

We review the main results achieved in the analysis of the stability and accuracy of the discrete least-squares approximation on multivariate polynomial spaces, with noiseless evaluations at random points [1], noiseless evaluations at low-discrepancy point sets [2], and noisy evaluations at random points [1,3].

References

1. A. Chkifa, A. Cohen, G. Migliorati, F. Nobile, R. Tempone: Discrete least squares polynomial approximation with random evaluations - application to parametric and stochastic elliptic PDEs, ESAIM Math. Model. Numer. Anal., 49(3):815-837, 2015.
2. G. Migliorati, F. Nobile: Analysis of discrete least squares on multivariate polynomial spaces with evaluations at low-discrepancy point sets, J. Complexity, 31(4):517-542, 2015.
3. G. Migliorati, F. Nobile, R.Tempone: Convergence estimates in probability and in expectation for discrete least squares with noisy evaluations at random points, J. Multivar. Anal., 142:167-182, 2015.

Giovanni Migliorati
Université Pierre et Marie Curie, Paris, France
e-mail: giovanni.migliorati@epfl.ch, giovanni.migliorati@gmail.com

Two numerical methods for mean-field games

Diogo Gomes

Here, we consider numerical methods for stationary mean-field games (MFG) and investigate two classes of algorithms. The first one is a gradient flow method based on the variational characterization of certain MFG. The second one uses monotonicity properties of MFG. We illustrate our methods with various examples, including one-dimensional periodic MFG, congestion problems, and higher-dimensional models.

Diogo Gomes
Computer, Electrical and Mathematical Sciences & Engineering Division King Abdullah University of Science and Technology (KAUST), Saudi Arabia
e-mail: diego.gomes@kaust.edu.sa

Comparison of stochastic programming and robust optimization approaches for risk management in energy generation

Ricardo Lima Antonio Conejo, Ibrahim Hoteit, Omar Knio and Sabique Langodan

We will discuss three optimization algorithms based on stochastic programming, robust optimization, and a hybrid method based on the two first methods. These algorithms are applied to a decision making problem for the scheduling and market involvement of a virtual power plant (VPP). This VPP operates a mix-energy system with thermal, hydro, and wind sources. The wind power and the electricity prices are uncertain and quantified by scenarios or convex sets. The methods are implemented using parallel optimization runs. The computational performance, scheduling results, and the impact of risk management are presented and discussed.

Ricardo Lima Ibrahim Hoteit, Omar Knio and Sabique Langodan
Computer, Electrical and Mathematical Sciences & Engineering Division King Abdullah University of Science and Technology (KAUST), Saudi Arabia
e-mail: {ricardo.lima,ibrahim.hoteit,sabique.langodan}@kaust.edu.sa,

Antonio Conejo
The Ohio State University, 286 Baker Systems Engineering, 1971 Neil Avenue, Columbus OH 43210, USA,
e-mail: conejonavarro.1@osu.edu

SDE based regression for random PDEs

Christian Bayer

A simulation based method for the numerical solution of PDE with random coefficients is presented. By the Feynman-Kac formula, the solution can be represented as conditional expectation of a functional of a corresponding stochastic differential equation driven by independent noise. A time discretization of the SDE for a set of points in the domain and a subsequent Monte Carlo regression lead to an approximation of the global solution of the random PDE. We provide an initial error and complexity analysis of the proposed method along with numerical examples illustrating its behaviour.

Christian Bayer
Weierstrass Institute for Applied Analysis and Stochastics, Berlin Germany
e-mail: christian.bayer@wias-berlin.de, christian.bayer1979@gmail.com

Uncertainty quantification for mean field games in social interactions

Ben Mansour Dia

We present an overview of mean field games formulation. A comparative analysis of the optimality for a stochastic McKean-Vlasov process with time-dependent probability is presented. Then we examine mean-field games for social interactions and we show that optimizing the long-term well-being through effort and social feeling state distribution (mean-field) will help to stabilize couple (marriage). However , if the cost of effort is very high, the couple fluctuates in a bad feeling state or the marriage breaks down. We then examine the influence of society on a couple using mean field sentimental games. We show that, in mean-field equilibrium, the optimal effort is always higher than the one-shot optimal effort. Finally we introduce the Wiener chaos expansion for the construction of solution of stochastic differential equations of Mckean-Vlasov type. The method is based on the Cameron-Martin version of the Wiener Chaos expansion and allow to quantify the uncertainty in the optimality system.

Ben Mansour Dia
Computer, Electrical and Mathematical Sciences & Engineering Division King Abdullah University of Science and Technology (KAUST), Saudi Arabia
e-mail: benmansour.dia@kaust.edu.sa

Poster session I

Sampling methods

I-1

Multi-Index Monte Carlo

Abdul–Lateef Haji–Ali, Fabio Nobile, and Raúl Tempone

We propose and analyze a novel Multi-Index Monte Carlo (MIMC) method for weak approximation of stochastic models that are described in terms of differential equations either driven by random measures or with random coefficients. The MIMC method is both a stochastic version of the combination technique introduced by Zenger, Griebel and collaborators and an extension of the Multilevel Monte Carlo (MLMC) method first described by Heinrich and Giles. Inspired by Giles's seminal work, instead of using first-order differences as in MLMC, we use in MIMC high-order mixed differences to reduce the variance of the hierarchical differences dramatically. Under standard assumptions on the convergence rates of the weak error, variance and work per sample, the optimal index set turns out to be of Total Degree (TD) type. When using such sets, MIMC yields new and improved complexity results, which are natural generalizations of Giles's MLMC analysis, and which increase the domain of problem parameters for which we achieve the optimal convergence, $\mathcal{O}(\mathrm{TOL}^{-2})$.

References:

1. Abdul–Lateef Haji–Ali, Fabio Nobile, Raúl Tempone, *Multi-Index Monte Carlo: When Sparsity Meets Sampling*, http://arxiv.org/abs/1405.3757, submitted to Numerische Mathematik in 2014.

Abdul–Lateef Haji–Ali and Raúl Tempone
King Abdullah University of Science and Technology, Thuwal, Saudi Arabia.
e-mail: abdullateef.hajiali@kaust.edu.sa, raul.tempone@kaust.edu.sa

Fabio Nobile
Ecole Polytechnique Fédérale de Lausanne, Switzerland.
e-mail: fabio.nobile@epfl.ch

I-2

Multi-index stochastic collocation for random elliptic PDEs

Abdul–Lateef Haji–Ali, Lorenzo Tamellini, Fabio Nobile, and Raúl Tempone

In this work we introduce the Multi-Index Stochastic Collocation method (MISC) for computing statistics of the solution of a PDE with random data. MISC is a combination technique based on mixed differences of spatial approximations and quadratures over the space of random data. We propose an optimization procedure to select the most effective mixed differences to include in the MISC estimator: such optimization is a crucial step and allows us to build a method that, provided with sufficient solution regularity, is potentially more effective than other multi-level collocation methods already available in literature. We then provide a complexity analysis that assumes decay rates of product type for such mixed differences, showing that in the optimal case the convergence rate of MISC is only dictated by the convergence of the deterministic solver applied to a one dimensional problem. We show the effectiveness of MISC with some computational tests, comparing it with other related methods available in the literature, such as the Multi-Index and Multilevel Monte Carlo, Multilevel Stochastic Collocation, Quasi Optimal Stochastic Collocation and Sparse Composite Collocation methods.

Abdul–Lateef Haji–Ali and Raúl Tempone
King Abdullah University of Science and Technology, Thuwal, Saudi Arabia.
e-mail: abdullateef.hajiali@kaust.edu.sa, raul.tempone@kaust.edu.sa

Lorenzo Tamellini
Department of Mathematics, Universit di Pavia, Italy

Fabio Nobile
Ecole Polytechnique Fédérale de Lausanne, Switzerland.
e-mail: fabio.nobile@epfl.ch

I-3

Hybrid Chernoff Tau-Leap

Alvaro Moraes, Raúl Tempone and Pedro Vilanova

Markovian pure jump processes can model many phenomena, e.g. chemical reactions at molecular level, protein transcription and translation, spread of epidemics diseases in small populations and in wireless communication networks among many others. In this work we present a novel hybrid algorithm for simulating individual trajectories which adaptively switches between the Stochastic Simulation Algorithm and the *Chernoff* Tau-leap Algorithm. This allows us to: (a) control the global exit probability of any simulated trajectory, (b) obtain accurate and computable estimates for the expected value of any smooth observable of the process with minimal computational work.

References:

1. A. Moraes, P. Vilanova and R. Tempone, "Hybrid Chernoff Tau-Leap", *SIAM Multiscale Modeling and Simulation*, Vol. 12, Issue 2, (2014).

Alvaro Moraes, Raúl Tempone and Pedro Vilanova
Computer, Electrical and Mathematical Sciences & Engineering Division King Abdullah University of Science and Technology (KAUST), Saudi Arabia
e-mail: {alvaro.moraesgutierrez,raul.tempone,pedro.guerra}@kaust.edu.sa

I-4

Multilevel Hybrid Chernoff Tau-Leap

Alvaro Moraes, Raúl Tempone and Pedro Vilanova

Markovian pure jump processes can model many phenomena, e.g. chemical reactions at molecular level, protein transcription and translation, spread of epidemics diseases in small populations and in wireless communication networks, among many others. In this work, we present a novel Multilevel Monte Carlo algorithm based on our *Chernoff Hybrid Tau-leap* method for path-simulation of continuous time Markov pure jump processes. This multilevel approach can be viewed as a variance reduction technique that allows us to obtain accurate and computable estimates for the expected value of any smooth observable of the process with minimal computational work.

References:

1. A. Moraes, P. Vilanova and R. Tempone, "Hybrid Chernoff Tau-Leap", *SIAM Multiscale Modeling and Simulation*, Vol. 12, Issue 2, (2014).

Alvaro Moraes, Raúl Tempone and Pedro Vilanova
Computer, Electrical and Mathematical Sciences & Engineering Division King Abdullah University of Science and Technology (KAUST), Saudi Arabia
e-mail: {alvaro.moraesgutierrez,raul.tempone,pedro.guerra}@kaust.edu.sa

I-5

Quasi-optimal sparse-grid approximations for random elliptic PDEs

Fabio Nobile, Lorenzo Tamellini, Raúl Tempone

In this poster we illustrate a possible strategy to minimize the impact of the "curse of dimensionality" effect when building sparse-grid approximations of a multivariate function $u = u(y_1, \ldots, y_N)$. More precisely, we will consider a "knapsack approach", in which we estimate the cost and the "error reduction" contribution of each possible component of the sparse grid, and then we choose the components with the highest "error reduction"/cost ratio. The estimates of the "error reduction" are obtained by a mixed "a-priori"/"a-posteriori" approach, in which we first derive a theoretical bound and then tune it with some inexpensive auxiliary computations.

This method is very general and can be used to build sparse grids either on bounded or unbounded domains (e.g. u depending on uniform and normal random distributions for y_n), using both nested and non-nested families of univariate collocation points (e.g. Clenshaw–Curtis, Leja, Genz–Keister, Gauss–Legendre or Gauss–Hermite points). We present some theoretical convergence results as well as numerical results showing the efficiency of the proposed approach for the approximation of the solution of elliptic PDEs with random diffusion coefficients.

References:

1. Nobile, F., Tamellini, L., Tempone, R.: Convergence of quasi-optimal sparse-grid approximation of Hilbert-space-valued functions: application to random elliptic PDEs. Accepted for publication on Numerische Mathematik, doi:10.1007/s00211-015-0773-y
2. Beck, J., Nobile, F., Tamellini, L., Tempone, R.: A Quasi-optimal Sparse Grids Procedure for Groundwater Flows. In: Spectral and High Order Methods for Partial Differential Equations - ICOSAHOM 2012, *Lecture Notes in Computational Science and Engineering*, vol. 95, pp. 1–16. Springer (2014).
3. Beck, J., Nobile, F., Tamellini, L., Tempone, R.: On the optimal polynomial approximation of stochastic PDEs by Galerkin and collocation methods. Mathematical Models and Methods in Applied Sciences **22**(09) (2012).

Fabio Nobile
MATHICSE-CSQI, École Polytechnique Fédérale de Lausanne, Switzerland,
e-mail: fabio.nobile@epfl.ch

Lorenzo Tamellini
Dipartimento di Matematica "F. Casorati", Università di Pavia, Italy,
e-mail: lorenzo.tamellini@unipv.it

Raul Tempone
Division of Computer, Electrical and Mathematical Sciences &Engineering, King Abdullah University of Science and Technology, Saudi Arabia
e-mail: raul.tempone@kaust.edu.sa

I-6

An adaptive sparse grid algorithm for elliptic PDEs with lognormal diffusion coefficient

Fabio Nobile, Lorenzo Tamellini, Raúl Tempone, Francesco Tesei

In this work (see [1]) we build on the classical adaptive sparse grid algorithm [5], obtaining an enhanced version capable of using non-nested collocation points, and supporting quadrature and interpolation on unbounded sets. We also consider several profit indicators that are suitable to drive the adaptation process. We then use such algorithm to solve an important test case in Uncertainty Quantification problem, namely the Darcy equation with lognormal permeability random field, and compare the results with those obtained with the quasi-optimal sparse grids based on profit estimates, which we have proposed in our previous works, cf. e.g. [3,4]. To treat the case of rough permeability fields, in which a sparse grid approach may not be suitable, we propose to use the adaptive sparse grid quadrature as a control variate in a Monte Carlo simulation, see also [2]. Numerical results show that the adaptive sparse grids have performances similar to those of the quasi-optimal sparse grids and are very effective in the case of smooth permeability fields. Moreover, their use as control variate in a Monte Carlo simulation allows to tackle efficiently also problems with rough coefficients, significantly improving the performances of a standard Monte Carlo scheme.

References:

1. Nobile, F., Tesei, F.: A Multi Level Monte Carlo Method with Control Variate for elliptic PDEs with log-normal coefficients. Stochastic Partial Differential Equations: Analysis and Computations, 3(3), 2015.
2. Nobile, F., Tamellini, L., Tempone, R.: Convergence of quasi-optimal sparse-grid approximation of Hilbert-space-valued functions: application to random elliptic PDEs. Accepted for publication on Numerische Mathematik, doi:10.1007/s00211-015-0773-y
3. Beck, J., Nobile, F., Tamellini, L., Tempone, R.: A Quasi-optimal Sparse Grids Procedure for Groundwater Flows. In: Spectral and High Order Methods for Partial Differential Equations - ICOSAHOM 2012, *Lecture Notes in Computational Science and Engineering*, vol. 95, pp. 1–16. Springer (2014).
4. Gerstner, T., Griebel, M. : Dimension-adaptive tensor-product quadrature, Computing 71, 2003.

Fabio Nobile · Francesco Tesei
MATHICSE-CSQI, École Polytechnique Fédérale de Lausanne, Switzerland.
e-mail: fabio.nobile, francesco.tesei @epfl.ch

Lorenzo Tamellini
Dipartimento di Matematica "F. Casorati", Università di Pavia, Italy,
e-mail: lorenzo.tamellini@unipv.it

Raúl Tempone
Division of Computer, Electrical and Mathematical Sciences & Engineering, King Abdullah University of Science and Technology, Saudi Arabia
e-mail: raul.tempone@kaust.edu.sa

I-7

Multilevel adaptive reaction-splitting simulation method for stochastic reaction networks

Alvaro Moraes, Raúl Tempone and Pedro Vilanova

This work is a generalization of our Multilevel Chernoff Tau-leap method that allow us to accurately estimate averages of observables of Stochastic Reaction Networks. Here, we adaptively split the set of reactions into two categories: fast and slow. Fast reactions are simulated by the Chernoff tau-leap method, while the slow ones are simulated using the modified next reaction method by D. Anderson. This approach defines a mixed method of approximate path simulation. By introducing a hierarchy of time discretization levels, we first show how to couple two mixed paths. Then, we define a Multilevel Monte Carlo estimator for the expected value of any observable based on the state of the process at a fixed final time T.

References:

1. A. Moraes, P. Vilanova and R. Tempone, "Hybrid Chernoff Tau-Leap", *SIAM Multiscale Modeling and Simulation*, Vol. 12, Issue 2, (2014).
2. A. Moraes, P. Vilanova and R. Tempone, "Multilevel Hybrid Chernoff Tau-Leap", *preprint arXiv:1403.2943*, (2014).

Alvaro Moraes, Raúl Tempone and Pedro Vilanova
Computer, Electrical and Mathematical Sciences & Engineering Division King Abdullah University of Science and Technology (KAUST), Saudi Arabia
e-mail: {alvaro.moraesgutierrez,raul.tempone,pedro.guerra}@kaust.edu.sa

I-8

Convergence estimates for discrete least-squares approximation with noisy evaluations at random points

Giovanni Migliorati, Fabio Nobile and Raúl Tempone.

we have proven convergence estimates in probability and in expectation for discrete least-squares approximations with noisy evaluations at random points, with several types of noise models. This poster presents the main steps in the proofs of these estimates, which have been obtained by combining results from the theory of large deviations, probability union bounds, and results from previous analyses

Giovanni Migliorati
Université Pierre et Marie Curie, France

Fabio Nobile
MATHICSE-CSQI, École Polytechnique Fédérale de Lausanne, Switzerland.
e-mail: fabio.nobile@epfl.ch

Raúl Tempone
Division of Computer, Electrical and Mathematical Sciences & Engineering, King Abdullah University of Science and Technology, Saudi Arabia
e-mail: raul.tempone@kaust.edu.sa

I-9

Multilevel Drift-Implicit Tau-Leap

Chiheb Ben Hammouda, Alvaro Moraes and Raúl Tempone

The dynamics of biochemical reactive systems with small copy numbers of one or more reactant molecules is dominated by stochastic effects. For those systems, discrete state-space and stochastic simulation approaches were proved to be more relevant than continuous state-space and deterministic ones. In systems characterized by having simultaneously fast and slow timescales, the existing discrete space-state stochastic path simulation methods such as the stochastic simulation algorithm (SSA) and the explicit tau- leap method can be very slow. Implicit approximations were developed in the literature to improve numerical stability and provide efficient simulation algorithms for those systems. In this work, we propose an efficient Multilevel Monte Carlo method in the spirit of the work by Anderson and Higham (2012) that uses drift-implicit tau-leap approximations at levels where the explicit tau-leap method is not applicable due to numerical stability issues. We present numerical examples that illustrate the performance of the proposed method.

Chiheb Ben Hammouda, Alvaro Moraes · Raúl Tempone
Division of Computer, Electrical and Mathematical Sciences & Engineering, King Abdullah University of Science and Technology, Saudi Arabia
e-mail: {chiheb.benhammouda, alvaro.moraesgutierrez,raul.tempone}@kaust.edu.sa

I-10

Optimal Hierarchies in Multilevel Monte Carlo

Abdul-Lateef Haji-Ali, Fabio Nobile, Erik von Schwerin, Raúl Tempone

We show the results of a general optimization of the parameters in the Multilevel Monte Carlo (MLMC) discretization hierarchy based on uniform discretization methods with general approximation orders and computational costs. We optimized hierarchies with geometric and non-geometric sequences of mesh sizes and showed that geometric hierarchies, when optimized, are nearly optimal and have the same asymptotic computational complexity as non-geometric optimal hierarchies. We discuss how enforcing constraints on parameters of MLMC hierarchies affects the optimality of these hierarchies. These constraints include an upper and a lower bound on the mesh size or enforcing that the number of samples and the number of discretization elements are integers. We also discuss the non-trivial optimal tolerance splitting between the bias and the statistical error contributions and its asymptotic behavior. The theoretical results are illustrated with two numerical examples using the Continuation MLMC Algorithm, and are shared with the poster with that title.

Abdul-Lateef Haji-Ali · Raúl Tempone
Division of Computer, Electrical and Mathematical Sciences & Engineering, King Abdullah University of Science and Technology, Saudi Arabia
e-mail: abdullateef.hajiali@kaust.edu.sa, raul.tempone@kaust.edu.sa

Fabio Nobile
MATHICSE-CSQI, École Polytechnique Fédérale de Lausanne, Switzerland.
e-mail: fabio.nobile@epfl.ch

Erik von Schwerin

I-11

A continuation Multilevel Monte Carlo

Nathan Collier, Abdul-Lateef Haji-Ali, Fabio Nobile, Erik von Schwerin, Raúl Tempone

We describe a novel Continuation Multi Level Monte Carlo (CMLMC) algorithm for weak approximation of stochastic models. The CMLMC algorithm solves the given approximation problem for a sequence of decreasing tolerances, ending when the required error tolerance is satisfied. CMLMC assumes discretization hierarchies that are defined a priori for each level and are geometrically refined across levels. The actual choice of computational work across levels is based on parametric models for the average cost per sample and the corresponding variance and weak error. These parameters are calibrated using Bayesian estimation, taking particular notice of the deepest levels of the discretization hierarchy, where only few realizations are available to produce the estimates. Numerical results substantiate the key results presented in the poster "Optimal Hierarchies in Multilevel Monte Carlo" and our claims about asymptotic normality of the statistical error in the MLMC estimator. The first example considers a three-dimensional elliptic partial differential equation with random inputs. Its space discretization is based on continuous piecewise trilinear finite elements and the corresponding linear system is solved by either a direct or an iterative solver. The second example considers a one-dimensional Ito stochastic differential equation discretized by a Milstein scheme.

Nathan Collier · Abdul-Lateef Haji-Ali · Raúl Tempone
Division of Computer, Electrical and Mathematical Sciences & Engineering, King Abdullah University of Science and Technology, Saudi Arabia
e-mail: abdullateef.hajiali@kaust.edu.sa, raul.tempone@kaust.edu.sa

Fabio Nobile
MATHICSE-CSQI, École Polytechnique Fédérale de Lausanne, Switzerland.
e-mail: fabio.nobile@epfl.ch

Erik von Schwerin

Poster session II

Bayesian Inference and Filtering

II-1

Bayesian inference and model comparison for metallic fatigue data

Ivo Babuška, Zaid Sawlan, Marco Scavino, Barna Szabó and Raúl Tempone

In this work, we present a statistical treatment of stress-life (S-N) data drawn from a collection of records of fatigue experiments that were performed on 75S-T6 aluminum alloys. Our main objective is to predict the fatigue life of materials by providing a systematic approach to model calibration, model selection and model ranking with reference to S-N data. To this purpose, we consider fatigue-limit models and random fatigue-limit models that are specially designed to allow the treatment of the run-outs (right-censored data). We first fit the models to the data by maximum likelihood methods and estimate the quantiles of the life distribution of the alloy specimen. To assess the robustness of the estimation of the quantile functions, we obtain bootstrap confidence bands by stratified resampling with respect to the cycle ratio. We then compare and rank the models by classical measures of fit based on information criteria. We also consider a Bayesian approach that provides, under the prior distribution of the model parameters selected by the user, their simulation-based posterior distributions. We implement and apply Bayesian model comparison methods, such as Bayes factor ranking and predictive information criteria based on cross-validation techniques under various a priori scenarios.

Ivo Babuška
ICES, The University of Texas at Austin, Austin, USA
e-mail: babuska@ices.utexas.edu

Zaid Sawlan, Marco Scavino and Raúl Tempone
CEMSE, King Abdullah University of Science and Technology, Thuwal, KSA
e-mail: zaid.sawlan@kaust.edu.sa,marco.scavino@kaust.edu.sa ,raul.tempone@kaust.edu.sa

Barna Szabó
Universidad de la República, Montevideo, Uruguay and Washington University in St. Louis, St. Louis, USA
e-mail: szabo@wustl.edu

II-2

Multilevel ensemble kalman filter

Håkon Hoel, Kody Law, Fabio Nobile, Alexey Chernov and Raúl Tempone

In this work we have combined the ideas of multilevel Monte Carlo and ensemble Kalman filtering (EnKF) to construct the multilevel ensemble Kalman filter (MLEnKF) for the setting of finite dimensional state and observation spaces. The main ideas of this method is to compute particle paths on a hierarchy of resolutions and to apply multilevel estimators on the ensemble hierarchy of particles to compute Kalman filter means and covariances. Theoretical and numerical results of the performance gains of MLEnKF over EnKF is presented and we also include some ideas on the extension of MLEnKF to settings with infinite dimensional state spaces.

Håkon Hoel
University of Oslo, Norway
e-mail: haakonah1@gmail.com

Kody Law
Oak Ridge National Lab, USA,
e-mail: lawkj@ornl.gov

Fabio Nobile
Ecole Polytechnique Fédérale de Lausanne, Switzerland.
e-mail: fabio.nobile@epfl.ch

Alexey Chernov · Raúl Tempone
CEMSE, King Abdullah University of Science and Technology, Thuwal, KSA
e-mail: raul.tempone@kaust.edu.sa

II-3

Multilevel sequential Monte Carlo samplers

Kody Law

This poster will review the probabilistic formulation of the inverse problem, the sequential Monte Carlo (SMC) sampling framework, and the standard multilevel Monte Carlo (MLMC) framework. These ideas will coalesce into the MLSMC sampling algorithm for Bayesian inverse problems. A numerical example of permeability inversion through an elliptic PDE given observations of pressure will illustrate the theoretical results.

Kody Law
Computer Science and Mathematics Division Oak Ridge National Laboratory Oak Ridge, TN, USA
e-mail: kodylaw@gmail.com

II-4

Solving inverse problem via non-linear update of gPCE coefficients

Alexander Litvinenko, Elmar Zander, Bojana Rosić and Hermann G. Matthies

A cheap approximation of the Bayesian Update (BU) is quite vital for uncertainty quantification. With BU we can take into account the given measurements of our physical model and update a priori probability density function (which is very often far away from the truth) of the uncertain parameter. The standard full BU is based on sampling and sampling is not always acceptable or possible. In addition, it can require a very large number of samples and is expensive. This motivated us to develop non-linear extension of the well-known Kalman filter, which we call non-linear Bayesian update (NLBU). We derive it from the minimum mean square error estimation. The idea is to get the update formula for generalized Polynomial Chaos coefficients and not only for the mean and covariance. We demonstrate few examples: diffusion PDE with uncertain permeability coefficient and a chaotic Lorenz 84 model with random coefficients.

References

1. H.G. Matthies, E. Zander, B.V. Rosić, A. Litvinenko, O. Pajonk, *Inverse Problems in a Bayesian Setting*, http://arxiv.org/pdf/1511.00524.pdf, 2015
2. A. Litvinenko, H. G. Matthies, *Inverse problems and uncertainty quantification*, http://arxiv.org/abs/1312.5048, 2013
3. B. V. Rosić A. Kucerová, J. Sýkora, O. Pajonk, A. Litvinenko, H. G. Matthies, *Parameter Identification in a Probabilistic Setting*, Engineering Structures, Vol. 50, pp 179-196, Elsevier, 2013
4. O. Pajonk, B.V. Rosić, A. Litvinenko, H.G. Matthies, *A deterministic filter for non-Gaussian Bayesian estimation - Applications to dynamical system estimation with noisy measurements*, Physica D: Nonlinear Phenomena 241 (7), 775-788, 2012
5. B.V. Rosić, A. Litvinenko, O. Pajonk, H. G. Matthies, *Sampling-free linear Bayesian update of polynomial chaos representations*, Journal of Computational Physics 231 (17), 5761-5787, 2012
6. A. Litvinenko, H.G. Matthies, *Uncertainty Quantification and Non-Linear Bayesian Update of PCE Coefficients*, PAMM 13 (1), 379-380, 2013
7. H.G.Matthies, A.Litvinenko, O.Pajonk, B.V.Rosić, E.Zander, *Parametric and uncertainty computations with tensor product representations*, Uncertainty Quantification in Scientific Com- puting, 139-150, (2012).
8. E. Zander, *Stochastic Galerkin library*, https://github.com/ezander/sglib
9. O. G. Ernst, B. Sprungk, H.-J. Starkloff, *Analysis of the Ensemble and Polynomial Chaos Kalman Filters in Bayesian Inverse Problems*, SIAM/ASA JUQ 3(1), (2015)

Alexander Litvinenko
Division of Computer, Electrical and Mathematical Sciences and Engineering
King Abdullah University of Science and Technology, Saudi Arabia.
e-mail: alexander.litvinenko@kaust.edu.sa

Elmar Zander, Bojana Rosić and Hermann G. Matthies
Technische Universität Braunschweig, Germany.
e-mail: h.matthies, ezander, bojana.rosic@tu-braunschweig.de

II-5

Hierarchical matrix approximation of large covariance matrices

Alexander Litvinenko, Marc Genton and Ying Sun

The class of Matérn covariance functions becomes very popular in spatial statistics and especially in geostatistics. We assume that there is a vector of measurements with a covariance matrix $C(\sigma^2, \nu, \ell)$ with uncertain variance σ^2, smoothness parameter ν and covariance length ℓ. The task is to use measurements to estimate uncertain parameters (σ^2, ν, ℓ). We do it by maximizing the log-likelihood function. On each iteration i of the maximization algorithm we need to (re)computed the covariance matrix C for a new/current parameter set. To speed up the solution of the optimization problem we approximate the covariance matrix by the hierarchical ($\mathcal{H}$)-matrix technique. The $\mathcal{H}$-matrix format has a log-linear computational cost and storage $\mathcal{O}(kn \log n)$, where rank $k \ll n$ is a small integer.

References

1. B. N. Khoromskij, A. Litvinenko, H. G. Matthies, *Application of hierarchical matrices for computing the Karhunen-Loéve expansion*, Computing, Vol. 84, Issue 1-2, pp 49-67, 2009, Springer Vienna
2. B. N. Khoromskij, A. Litvinenko, *Data Sparse Computation of the Karhunen-Loéve Expansion*, International Conference on Numerical Analysis and Applied Mathematics 2008, Vol. 1048, Issue 1, pp 311-314, AIP Publishing
3. W. Nowak, A. Litvinenko, *Kriging and Spatial Design Accelerated by Orders of Magnitude: Combining Low-Rank Covariance Approximations with FFT-Techniques*, Mathematical Geosciences, Vol. 45, Issue 4, pp.411-435, 2013
4. H.G. Matthies, E. Zander, B.V. Rosić, A. Litvinenko, O. Pajonk, *Inverse Problems in a Bayesian Setting*, http://arxiv.org/pdf/1511.00524.pdf, 2015
5. A. Litvinenko, H. G. Matthies, *Inverse problems and uncertainty quantification*, http://arxiv.org/abs/1312.5048, 2013
6. B. V. Rosić A. Kucerová, J. Sýkora, O. Pajonk, A. Litvinenko, H. G. Matthies, *Parameter Identification in a Probabilistic Setting*, Engineering Structures, Vol. 50, pp 179-196, Elsevier, 2013
7. O. Pajonk, B.V. Rosić, A. Litvinenko, H.G. Matthies, *A deterministic filter for non-Gaussian Bayesian estimation - Applications to dynamical system estimation with noisy measurements*, Physica D: Nonlinear Phenomena 241 (7), 775-788, 2012
8. B.V. Rosić, A. Litvinenko, O. Pajonk, H. G. Matthies, *Sampling-free linear Bayesian update of polynomial chaos representations*, Journal of Computational Physics 231 (17), 5761-5787, 2012
9. A. Litvinenko, H.G. Matthies, *Uncertainty Quantification and Non-Linear Bayesian Update of PCE Coefficients*, PAMM 13 (1), 379-380, 2013
10. H.G.Matthies, A.Litvinenko, O.Pajonk, B.V.Rosić, E.Zander, *Parametric and uncertainty computations with tensor product representations*, Uncertainty Quantification in Scientific Computing, 139-150, (2012).

A.Litvinenko
SRI UQ and ECRC, Division of Computer, Electrical, and Mathematical Science and Engineering, King Abdullah University of Science and Technology , Thuwal, Saudi Arabia.
e-mail: alexander.litvinenko@kaust.edu.sa

M. Genton
CEMSE Division, King Abdullah University of Science and Technology, Thuwal, Saudi Arabia.
e-mail: marc.genton@kaust.edu.sa

Ying Sun
CEMSE Division, King Abdullah University of Science and Technology, Thuwal, Saudi Arabia.
e-mail: ying.sun@kaust.edu.sa

II-6

Multiscale Modeling of Wear Degradation

Alvaro Moraes, Fabrizio Ruggeri, Raúl Tempone and Pedro Vilanova

Cylinder liners of diesel engines used for marine propulsion are naturally subjected to a wear process, and may fail when their wear exceeds a specified limit. Since failures often represent high economical costs, it is utterly important to predict and avoid them. In this work, we model the wear process using a pure jump process. Therefore, the inference goal here is to estimate: the number of possible jumps, its sizes, the coefficients and the shapes of the jump intensities. We propose a multiscale approach for the inference problem that can be seen as an indirect inference scheme. We found that using a Gaussian approximation based on moment expansions, it is possible to accurately estimate the jump intensities and the jump amplitudes. We obtained results equivalent to the state of the art but using a simpler and less expensive approach.

References:

1. A. Moraes, F. Ruggeri, P. Vilanova and R. Tempone, "Multiscale Modeling of Wear Degradation in Cylinder Liners", SIAM Multiscale Modeling and Simulation, Vol. 12, Issue 1 (2014).

Alvaro Moraes, , Raúl Tempone and Pedro Vilanova
Computer, Electrical and Mathematical Sciences & Engineering Division King Abdullah University of Science and Technology (KAUST), Saudi Arabia
e-mail: {alvaro.moraesgutierrez,raul.tempone,pedro.guerra}@kaust.edu.sa,

Fabrizio Ruggeri
CNR-IMATI, Milano, Italy
e-mail: fabrizio@mi.imati.cnr.it

II-7

Bayesian Inference for Linear Parabolic PDEs with Noisy Boundary Conditions

Fabrizio Ruggeri, Zaid Sawlan, Marco Scavino and Raúl Tempone

In this work we develop a Bayesian setting to infer unknown parameters in initial-boundary value problems related to linear parabolic partial differential equations. We realistically assume that the boundary data are noisy, for a given prescribed initial condition. We show how to derive the joint likelihood function for the forward problem, given some measurements of the solution field subject to Gaussian noise. Given Gaussian priors for the time-dependent Dirichlet boundary values, we analytically marginalize the joint likelihood using the linearity of the equation. Our hierarchical Bayesian approach is fully implemented in an example that involves the heat equation. In this example, the thermal diffusivity is the unknown parameter. We assume that the thermal diffusivity parameter can be modeled a priori through a lognormal random variable or by means of a space-dependent stationary lognormal random field. Synthetic data are used to test the inference. We exploit the behavior of the non-normalized log posterior distribution of the thermal diffusivity. Then, we use the Laplace method to obtain an approximated Gaussian posterior and therefore avoid costly Markov Chain Monte Carlo computations. Expected information gains and predictive posterior densities for observable quantities are numerically estimated using Laplace approximation for different experimental setups.

Fabrizio Ruggeri
CNR - IMATI, Consiglio Nazionale delle Ricerche, Milano, Italy
e-mail: fabrizio@mi.imati.cnr.it

Zaid Sawlan, Marco Scavino and Raúl Tempone
CEMSE, King Abdullah University of Science and Technology, Thuwal, KSA
e-mail: {zaid.sawlan,marco.scavino,raul.tempone}@kaust.edu.sa

Marco Scavino
Universidad de la República, Montevideo, Uruguay

II-8

An Efficient Forward-Reverse EM Algorithm for Statistical Inference in Stochastic Reaction Networks

Christian Bayer, Alvaro Moraes, Raúl Tempone and Pedro Vilanova

In this work, we present an extension to the context of Stochastic Reaction Networks (SRNs) of the forward-reverse representation introduced in "Simulation of forward-reverse stochastic representations for conditional diffusions", a 2014 paper by Bayer and Schoenmakers. We apply this stochastic representation in the computation of efficient approximations of expected values of functionals of SRN bridges, i.e, SRNs conditioned to their values in the extremes of given time-intervals. We then employ this SRN bridge-generation technique to the statistical inference problem of approximating the reaction propensities based on discretely observed data. To this end, we introduce a two-phase iterative inference method in which, during phase I, we solve a set of deterministic optimization problems where the SRNs are replaced by their reaction-rate Ordinary Differential Equations (ODEs) approximation; then, during phase II, we apply the Monte Carlo version of the Expectation-Maximization (EM) algorithm starting from the phase I output. By selecting a set of over dispersed seeds as initial points for phase I, the output of parallel runs from our two-phase method is a cluster of approximate maximum likelihood estimates. Our results are illustrated by numerical examples.

References:

1. Christian Bayer and John Schoenmakers "Simulation of Forward-reverse Stochastic Representations for Conditional Diffusions", Annals of Applied Probability, Vol. 24, Issue 5 (2014).
2. Christian Bayer, Alvaro Moraes, Raúl Tempone and Pedro Vilanova "An Efficient Forward-Reverse Expectation-Maximization Algorithm for Statistical Inference in Stochastic Reaction Networks", Accepted for publication in Stochastic Analysis and its Applications (2015).

Christian Bayer
Weierstrass Institute for applied analysis and stochastics, Berlin, Germany
e-mail: christian.bayer@wias-berlin.de

Alvaro Moraes, , Raúl Tempone and Pedro Vilanova
Computer, Electrical and Mathematical Sciences & Engineering Division King Abdullah University of Science and Technology (KAUST), Saudi Arabia
e-mail: {alvaro.moraesgutierrez,raul.tempone,pedro.guerra}@kaust.edu.sa,

II-9

Bayesian inference of the heat transfer properties of a wall using experimental data

Marco Iglesias, Zaid Sawlan, Marco Scavino, Raúl Tempone and Christopher Wood

A hierarchical Bayesian inference method is developed to estimate the thermal resistance and volumetric heat capacity of a wall. We apply our methodology to a real case study where measurements are recorded each minute from two temperature probes and two heat flux sensors placed on both sides of a solid brick wall along a period of almost five days. We model the heat transfer through the wall by means of the one-dimensional heat equation with Dirichlet boundary conditions. The initial/boundary conditions for the temperature are approximated by piecewise linear functions. We assume that temperature and heat flux measurements have independent Gaussian noise and derive the joint likelihood of the wall parameters and the initial/boundary conditions. Under the model assumptions, the boundary conditions are marginalized analytically from the joint likelihood. Approximated Gaussian posterior distributions for the wall parameters and the initial condition parameter are obtained using the Laplace method, after incorporating the available prior information. The information gain is estimated under different experimental setups, to determine the best allocation of resources.

Marco Iglesias
School of Mathematical Sciences, University of Nottingham, Nottingham NG7 2RD, UK

Zaid Sawlan, Marco Scavino and Raúl Tempone
CEMSE, King Abdullah University of Science and Technology, Thuwal, KSA
e-mail: {zaid.sawlan,marco.scavino,raul.tempone}@kaust.edu.sa

Marco Scavino
Universidad de la República, Montevideo, Uruguay

Christopher Wood
Department of Architecture and Built Environment, Faculty of Engineering, University of Nottingham, University Park, Nottingham NG7 2RD, UK

II-10

Fast Bayesian Optimal Experimental Design for Seismic Source Inversion

Quan Long, Mohammed Motamed and Raúl Tempone

We develop a fast method for optimally designing experiments in the context of statistical seismic source inversion . In particular, we efficiently compute the optimal number and locations of the receivers or seismographs. The seismic source is modeled by a point moment tensor multiplied by a time-dependent function. The parameters include the source location, moment tensor components, and start time and frequency in the time function. The forward problem is modeled by the elastic wave equations. We show that the Hessian of the cost functional, which is usually defined as the square of the weighted L2 norm of the difference between the experimental data and the simulated data, is proportional to the measurement time and the number of receivers. Consequently, the posterior distribution of the parameters, in a Bayesian setting, concentrates around the "true" parameters, and we can employ Laplace approximation and speed up the estimation of the expected Kullback-Leibler divergence (expected information gain), the optimality criterion in the experimental design procedure. Since the source parameters span several magnitudes, we use a scaling matrix for efficient control of the condition number of the original Hessian matrix. We use a second-order accurate finite difference method to compute the Hessian matrix and either sparse quadrature or Monte Carlo sampling to carry out numerical integration. We demonstrate the efficiency, accuracy, and applicability of our method on a two-dimensional seismic source inversion problem.

Quan Long
United Technologies Research Center, East Hartford, CT, USA
e-mail: longq@utrc.utc.com

Mohammed Motamed
Department of Mathematics and Statisitics, University of New Mexico, NM, USA
e-mail: motamed@math.unm.unm.edu

Raúl Tempone
Computer, Electrical and Mathematical Sciences & Engineering Division King Abdullah University of Science and Technology (KAUST), Saudi Arabia
e-mail: raul.tempone@kaust.edu.sa,

Poster session III

Stochastic Differential Equations

III-1

Indirect Inference for Stochastic Differential Equations Based on Moment Expansions

Marco Ballesio, Pedro Vilanova and Raúl Tempone

We provide an indirect inference method to estimate the parameters of scalar diffusion and jump diffusion processes. We obtain a system of ODEs for the time evolution of the first two moments of the process by the approximation of the stochastic model applying a second order Taylor expansion of the SDE's infinitesimal generator in the Dynkin's formula. This method allows a simple and efficient procedure to infer the parameters of such stochastic processes by the maximization of the likelihood of the approximating Gaussian process given the data. Finally, we perform numerical experiments for two datasets arising from organic and inorganic fouling deposition phenomena.

Marco Ballesio, Pedro Vilanova and Raúl Tempone
CEMSE, King Abdullah University of Science and Technology, Thuwal, KSA
e-mail: {pedro.vilanova,raul.tempone}@kaust.edu.sa
e-mail: marco.ballesio@outlook.it

III-2

Time-optimal path planning in uncertain flow fields using ensemble method

Tong Wang, Olivier P. Le Maître, Ibrahim Hoteit, and Omar M. Knio

An ensemble-based approach is developed to conduct time-optimal path planning in spatially complex, strong, time-varying ocean currents under uncertainty. Attention is restricted to two-dimensional steady and unsteady uncertain flows, yet the sampling methodology mimics situations arising in operational forecasts, where a set deterministic predictions is used to model and quantify uncertainty in the predictions. In the operational setting, much about dynamics, topography and forcing of the ocean environment is uncertain, and as a result a single path produced by a model simulation has limited utility. To overcome this limitation, we rely on a finite-size ensemble of deterministic forecasts to quantify the impact of variability in the dynamics. The uncertainty of flow field is parametrized using a finite number of independent canonical random variables with known densities, and the ensemble is generated by sampling these variables. For each the resulting realizations of the uncertain current field, we predict the "optimal" path by solving a boundary value problem (BVP), based on the Pontryagin maximum principle. A family of backward-in-time trajectories starting at the end position is used to generate suitable initial values for the BVP solver. This allows us to examine and analyze the performance of sampling strategy, and develop insight into extensions dealing with regional or general circulation models. In particular, the ensemble method enables us to perform a statistical analysis of travel times, and consequently develop a path planning approach that accounts for these statistics. The proposed methodology is tested for a number of scenarios. We first validate our algorithms by reproducing simple canonical solutions, and then demonstrate our approach in more complex flow fields, including idealized, steady and unsteady double-gyre flows.

T. Wang · I. Hoteit · O. M. Knio
Division of Computer, Electrical and Mathematical Sciences and Engineering, King Abdullah University of Science and Technology, Thuwal, Saudi Arabia
e-mail: Omar.Knio@kaust.edu.sa

O. P. Le Maître
LIMSI-CNRS, BP 133, 91403 Orsay, France

III-3

First order mean field games - explicit solutions, perturbations and connection with classical mechanics

Diogo Gomes, Levon Nurbekyan, Mariana Prazeres

In this poster, we present some recent developments in the theory of first order mean field games.

A standard assumption in mean field games is that the cost function of the agents is monotone in the density of the distribution of the agents. This assumption leads to a comprehensive theory of existence and uniqueness of smooth solutions. Our goal is to study the case when the potential is not monotone in the density. In this case, we construct non-unique explicit solutions for a broad class of first-order mean-field games. We observe non-uniqueness of the solutions and the breakdown of the regularity. These examples illustrate new phenomenon: the formation of regions with no agents.

Furthermore, under a local monotonicity assumption, we show that small perturbations of mean field games have unique smooth solutions. In addition, we explore the connection between first-order mean field games and classical mechanics and KAM theory.

Lastly, we provide an alternative formulation of mean-field game equations in terms of a new current variable. With this formulation, we obtain new identities and estimates.

Diogo Gomes, Levon Nurbekyan, Mariana Prazeres
CEMSE, King Abdullah University of Science and Technology, Thuwal, KSA
e-mail: diego.gomes@kaust.edu.sa

III-4

New a priori estimates for mean-field games with congestion

David Evangelista, Diogo Gomes

We present recent developments in crowd dynamics models (e.g. pedestrian flow problems). Our formulation is given by mean-field games with congestion that we consider both in time-dependent and in the stationary cases. We start by introducing basic models and present some extension and generalizations for stationary problems. We establish some new a priori estimates that give partial regularity of the solutions. We then finish with numerical results for an example for which our results apply.

References:

1. D. Gomes and H. Mitake. Stationary mean-field games with congestion and quadratic hamiltonians. Preprint
2. D. Gomes and V. Voskanyan. Short-time existence of solutions for mean-field games with congestion. Preprint

David Evangelista, Diogo Gomes
CEMSE, King Abdullah University of Science and Technology, Thuwal, KSA
e-mail: david.evangelista@kaust.edu.sa, diogo.gomes@kaust.edu.sa

III-5

Neuro-Inspired Computing with Stochastic Electronics

Rawan Naous, Maruan Al-Shedivat, Emre Neftci, Gert Cauwenberghs, and Khaled Salama

The extensive scaling and integration within electronic systems have set the standards for what is addressed to as stochastic electronics. Individual components are increasingly diverting away from their reliable behavior and producing undeterministic outputs. This stochastic operation highly mimics the biological medium within the brain. Hence, building on the inherent variability, particularly within novel non-volatile memory technologies, paves the way for unconventional neuromorphic designs. Neuro-inspired networks with brain-like structures of neurons and synapses allow for computations and levels of learning for diverse recognition tasks and applications.

Rawan Naous,
CEMSE, King Abdullah University of Science and Technology, Thuwal, KSA
e-mail: rawan.naous@kaust.edu.sa

III-6

Pricing under rough volatility

Christian Bayer

From an analysis of the time series of realized variance (RV) using recent high frequency data, Gatheral, Jaisson and Rosenbaum (2014) previously showed that log-RV behaves essentially as a fractional Brownian motion with Hurst exponent H of order 0.1, at any reasonable time scale. The resulting Rough Fractional Stochastic Volatility (RFSV) model is remarkably consistent with financial time series data. We now show how the RFSV model can be used to price claims on both the underlying and integrated variance. We analyze in detail a simple case of this model, the rBergomi model. In particular, we find that the rBergomi model fits the SPX volatility markedly better than conventional Markovian stochastic volatility models, and with fewer parameters. Finally, we show that actual SPX variance swap curves seem to be consistent with model forecasts, with particular dramatic examples from the weekend of the collapse of Lehman Brothers and the Flash Crash.

Christian Bayer
Weierstrass Institute for applied analysis and stochastics, Berlin, Germany
e-mail: christian.bayer@wias-berlin.de

III-7

A non-intrusive approach for PC analysis of SDEs driven by Wiener noise

Maria Navarro, Olivier Le Maître, Omar Knio

- Stochastic differential equations (SDEs) apply to different fields, such us: biology, finance, weather prediction, etc.
- Mathematical models will almost always have uncertain components (unknown parameters, imprecise experimental data, etc.)
- To analyze and simulate models based on SDEs in a reliable way, it is necessary to develop techniques which deal with the two sources of uncertainty (parametric and stochastic).
- Under the assumption that the Wiener noise and the uncertain parameters are independent, a PC analysis of SDEs with parametric uncertainty was proposed in [1].
- Problem: The PC modes were computed by Galerkin, but there are complex settings where the implementation of Galerkin is not feasible.

References:

1. O. Le Maître, O. Knio, PC analysis of stochastic differential equations driven by Wiener noise, Reliability Engineering & System Safety, 135, 107-124, 2015.
2. M. Navarro, O. Le Maître, O. Knio, A non-intrusive approach for PC analysis of stochastic differential equations driven by Wiener noise with uncertain parameters, In preparation.

Maria Navarro, Olivier Le Maître and Omar Knio
Weierstrass Institute for applied analysis and stochastics, Berlin, Germany
e-mail: christian.bayer@wias-berlin.de

Poster session IV

Green Wireless Communication

IV-1

Optimized energy efficiency and spectral efficiency resource allocation strategies for phantom cellular networks

Amr Mohamed Abdelaziz Abdelhady, Osama Amin and Mohamed Slim Alouini

Multi-tier heterogeneous networks have become an essential constituent for next generation cellular networks. Meanwhile, energy efficiency (EE) has been considered a critical design criterion along with the traditional spectral efficiency (SE) metric. In this context, we study power and spectrum allocation for the recently proposed two-tier architecture known as Phantom cellular networks. The optimization framework includes both EE and SE, where we propose an algorithm that computes the SE and EE resource allocation for Phantom cellular networks. Then, we compare the performance of both design strategies versus the number of users, and the ratio of Phantom cell resource blocks to the total number of resource blocks. We aim to investigate the effect of some system parameters to achieve improved SE or EE performance at a non-significant loss in EE or SE performance, respectively. It was found that the system parameters can be tuned so that the EE solution does not yield a significant loss in the SE performance.

Amr Mohamed Abdelaziz Abdelhady, Osama Amin and Mohamed Slim Alouini
Computer, Electrical and Mathematical Sciences & Engineering Division King Abdullah University of Science and Technology (KAUST), Saudi Arabia
e-mail: {amr.abdelhady,osama.amin,slim.alouini}@kaust.edu.sa

IV-2

Secure Broadcasting with Uncertain Channel State Information

Amal Hyadi, Zouheir Rezki, Mohamed-Slim Alouini

We investigate the problem of secure broadcasting over fast fading channels with imperfect main channel state information (CSI) at the transmitter. In particular, we analyze the effect of the noisy estimation of the main CSI on the throughput of a broadcast channel where the transmission is intended for multiple legitimate receivers in the presence of an eavesdropper. Besides, we consider the realistic case where the transmitter is only aware of the statistics of the eavesdropper's CSI and not of its channel's realizations. First, we discuss the common message transmission case where the source broadcasts the same information to all the receivers, and we provide an upper and a lower bounds on the ergodic secrecy capacity. For this case, we show that the secrecy rate is limited by the legitimate receiver having, on average, the worst main channel link and we prove that a non-zero secrecy rate can still be achieved even when the CSI at the transmitter is noisy. Then, we look at the independent messages case where the transmitter broadcasts multiple messages to the receivers, and each intended user is interested in an independent message. For this case, we present an expression for the achievable secrecy sum-rate and an upper bound on the secrecy sum-capacity and we show that, in the limit of large number of legitimate receivers K, our achievable secrecy sum-rate follows the scaling law $\log\left((1-\alpha)\log(K)\right)$, where α is the estimation error variance of the main CSI. The special cases of high SNR, perfect and no-main CSI are also analyzed. Analytical derivations and numerical results are presented to illustrate the obtained expressions for the case of independent and identically distributed Rayleigh fading channels.

References:

1. A. Hyadi, Z. Rezki, A. Khisti and M.-S. Alouini, "On the secrecy capacity of the broadcast wiretap channel with imperfect channel state information", in Proceedings of IEEE Global Communications Conference (Globecom?2014), Austin, TX, USA, Dec. 2014.
2. A. Hyadi, Z. Rezki, A. Khisti and M.-S. Alouini, "Secure Broadcasting with Imperfect Channel State Information at the Transmitter", submitted to IEEE Transactions on Wireless Communications.

Amal Hyadi, Zouheir Rezki, Mohamed-Slim Alouini
Division of Computer, Electrical, and Mathematical Sciences & Engineering (CEMSE), King Abdullah University of Science and Technology (KAUST), Thuwal, Makkah Province, Saudi Arabia.
e-mail: amal.hyadi, zouheir.rezki, slim.alouini@kaust.edu.sa

IV-3

Performance Analysis of Communications under Energy Harvesting Constraints with noisy CSI

Mohamed Ridha Zenaidi, Zouheir Rezki, Hamidou Tembine and Mohamed-Slim Alouini

In energy harvesting communications, the transmitters have to adapt transmission to availability of energy harvested during the course of communication. The performance of the transmission depends on the channel conditions which vary randomly due to mobility and environmental changes. In this work, we consider the problem of power allocation taking into account the energy arrivals over time and the degree of channel state information (CSI) available at the transmitter, in order to maximize the throughput. Differently from previous work, the CSI at the transmitter is not perfect and may include estimation errors. We solve this problem with respect to the Energy Harvesting constraints. We determine the optimal power policy in the case where the channel is assumed to be perfectly known at the receiver. Also, we obtain the power policy when the transmitter has no CSI. Furthermore, we analyze the asymptotic average throughput in a system where the average recharge rate goes asymptotically to zero and when it is very high.

References:

1. O. Ozel, K. Tutuncuoglu, J. Yang, S. Ulukus and A. Yener, "Transmission with Energy Harvesting Nodes in Fading Wireless Channels: Optimal Policies," *IEEE J.Select. Areas Commun.*,vol. 29, no. 8, pp.1732-1743, Sep. 2011.
2. C. Ho, and R. Zhang, "Optimal energy allocation for wireless communications with energy harvesting constraints," *IEEE Trans. Signal. Process.*,vol 60, no. 9, pp.4808-4818, Sep. 2012.
3. M.-R. Znaidi, Z. Rezki, H. Tembine, M.-S. Alouini, "Performance Limits of Energy Harvesting Communications under Imperfect Channel State Information," *Submitted to ICC'16.*

Mohamed Ridha Zenaidi, Zouheir Rezki and Mohamed-Slim Alouini
Electrical Engineering Program Computer, Electrical, and Mathematical science and Engineering (CEMSE) Division, King Abdullah University of Science and Technology (KAUST), Kingdom of Saudi Arabia
e-mail: mohamed.znaidi,zouheir.rezki,slim.alouini@kaust.edu.sa

Hamidou Tembine
Electrical and Computer Engineering New York University, Abu Dhabi, UAE
e-mail: tembine@nyu.edu

IV-4

Device-to-Device Underlay Cellular Networks with Uncertain Channel State Information

Amen Memmi, Zouheir Rezki and Mohamed-Slim Alouini

Device-to-Device (D2D) communications underlying the cellular infrastructure is a technology that has recently been proposed as a promising solution to enhance cellular network capabilities: It improves spectrum utilization, overall throughput and energy efficiency while enabling new peer-to-peer and location-based applications and services. However, interference is the major challenge since the same resources are shared by both systems. Therefore, interference management techniques are required to keep the interference under control. In this work, in order to mitigate interference, we consider centralized and distributed power control algorithms in a one-cell random network model. Differently from previous works, we are assuming that the channel state information (CSI) may be imperfect and include estimation errors. We evaluate how this uncertainty impacts performances.

References:

1. A. Memmi, Z. Rezki and M.-S. Alouini, "Power Control for D2D Underlay Cellular Networks with Imperfect CSI", submitted to IEEE ICC 2016.

Amen Memmi, Zouheir Rezki and Mohamed-Slim Alouini
Computer, Electrical, and Mathematical Sciences and Engineering (CEMSE) Division King Abdullah University of Science and Technology (KAUST), Saudi Arabia
e-mail: {amen.memmi,zouheir.rezki,slim.alouini}@kaust.edu.sa

IV-5

On the Symmetric α-Stable Distribution with Application to Symbol Error Rate Calculations

Hamza Soury and Mohamed-Slim Alouini

The probability density function (PDF) of the α-stable distribution is investigated using the inverse Fourier transform of its characteristic function. For general values of the stable parameter α, it is shown that the PDF of the symmetric stable distribution can be expressed in terms of the Fox H function and so is the cumulative distribution function. These new expressions are used to get the probability of error of single input single output communication systems using different modulation schemes in absence and presence of fading. Moreover, simpler expressions of these error rates are deduced for some selected special cases and compact approximations are derived using asymptotic expansions.

Hamza Soury and Mohamed-Slim Alouini
Computer, Electrical, and Mathematical Sciences and Engineering (CEMSE) Division King Abdullah University of Science and Technology (KAUST)
e-mail: {soury.hamza, slim.alouini}@kaust.edu.sa

IV-6

Performance Analysis of Coordination Strategies in Two-Tier Heterogenous Networks

Ikram Boukhedimi, Abla Kammoun, and Mohamed-Slim Alouini

Large scale multi-tier heterogeneous networks (HetNets) are expected to ensure a consistent quality of service (QoS) in 5G systems. Such networks consist of a macro base station (BS) equipped with a large number of antennas and a dense overlay of small cells. The small cells could be deployed within the same coverage of the macro-cell BS, thereby causing high levels of inter-cell interferences. In this regard, coordinated beamforming techniques are considered as a viable solution to counteract the arising interference. The goal of this work is to analyze the efficiency of coordinated beamforming techniques in mitigating both intra-cell and inter-cell interferences. In particular, we consider the downlink of a frequency-division duplexing (FDD) massive multiple-input-multiple-output (MIMO) tier-HetNet and analyze different beamforming schemes together with different degrees of coordination between the BSs. We exploit random matrix theory tools in order to provide, in explicit form, deterministic equivalents for the average achievable rates in the macro-cell and the micro-cells. We prove that our theoretical derivations allow us to draw some conclusions regarding the role played by coordination strategies in reducing the inter-cell interference. These findings are finally validated by a selection of some numerical results.

Ikram Boukhedimi, Abla Kammoun, and Mohamed-Slim Alouini
Computer, Electrical, and Mathematical Sciences and Engineering (CEMSE) Division, King Abdullah University of Science and Technology (KAUST),Thuwal, Makkah Province, Kingdom of Saudi Arabia.
e-mail: {ikram.boukhedimi, abla.kammoun, slim.alouini}@kaust.edu.sa

IV-7

A unified simulation approach for the fast outage capacity evaluation over generalized fading channels

Nadhir Ben Rached, Abla Kammoun, Mohamed-Slim Alouini, and Raúl Tempone

The outage capacity (OC) is among the most important performance metrics of communication systems over fading channels. The evaluation of the OC, when Equal Gain Combining (EGC) or Maximum Ratio Combining (MRC) diversity techniques are employed, boils down to computing the Cumulative Distribution Function (CDF) of the sum of channel envelopes (equivalently amplitudes) for EGC or channel gain (equivalently squared enveloped/amplitudes) for MRC. Closed-form expressions of the CDF of the sum of many generalized fading variates are generally unknown and constitute open problems. In this work, we develop a unified hazard rate twisting Importance Sampling (IS) based approach to efficiently estimate the CDF of the sum of independent arbitrary variates. The proposed IS estimator is shown to achieve an asymptotic optimality criterion, which clearly guarantees its efficiency. Some selected simulation results are also shown to illustrate the substantial computational gain achieved by the proposed IS scheme over crude Monte-Carlo simulations.

Nadhir Ben Rached, Abla Kammoun, Mohamed-Slim Alouini, Raúl Tempone
Computer, Electrical, and Mathematical Sciences and Engineering (CEMSE) Division, King Abdullah University of Science and Technology (KAUST),Thuwal, Makkah Province, Kingdom of Saudi Arabia.
e-mail: {nadhir.benrached, abla.kammoun, slim.alouini, raul.tempone}@kaust.edu.sa

IV-8

Polynomial Expansion of the Power Minimization Precoder in Large-Scale MIMO Systems

Houssem Sifaou, Abla Kammoun, Luca Sanguinetti, Mérouane Debbah and Mohamed-Slim Alouini

This work focuses on the downlink of a single-cell large-scale MIMO system in which the base station equipped with M antennas serves K single-antenna users. In particular, we are interested in reducing the implementation complexity of the optimal linear precoder (OLP) that minimizes the total power consumption while ensuring target user rates. As most precoding schemes, a major difficulty towards the implementation of OLP is that it requires fast inversions of large matrices in every coherence period. To overcome this issue, we aim at designing a linear precoding scheme providing the same performance of OLP but with lower complexity. This is achieved by applying the truncated polynomial expansion (TPE) concept on a per-user basis. To get a further leap in complexity reduction and allow for closed-form expressions of the per-user weighting coefficients, we resort to the asymptotic regime in which M and K grow large with a bounded ratio. Numerical results are used to show that the proposed TPE precoding scheme achieves the same performance of OLP with a significantly lower implementation complexity.

Houssem Sifaou, Abla Kammoun, Mohamed-Slim Alouini
CEMSE Division, King Abdullah University of Science and Technology, Thuwal, Saudi Arabia

Luca Sanguinetti
Dipartimento di Ingegneria dell'Informazione, University of Pisa, Pisa, Italy

Mérouane Debbah
Large Networks and System Group (LANEAS), Centrale Supélec, Université Paris-Saclay, Gif-sur-Yvette, France and Mathematical and Algorithmic Sciences Lab, Huawei France R&D, Paris, France.

IV-9

Sharing the Licensed Spectrum of Full-duplex Systems using Improper Gaussian Signaling

Mohamed Gaafar, Osama Amin, Walid Abediseid and Mohamed-Slim Alouini

Sharing the spectrum with in-band full-duplex (FD) primary users (PU) is a challenging and interesting problem in the underlay cognitive radio (CR) systems. The self-interference introduced at the primary network may dramatically impede the secondary user (SU) opportunity to access the spectrum. In this work, we attempt to tackle this problem through the use of the so-called improper Gaussian signaling. Such a signaling technique has demonstrated its superiority in improving the overall performance in interference limited networks. Particularly, we assume a system with a SU pair working in half-duplex mode that uses improper Gaussian signaling while the FD PU pair implements the regular proper Gaussian signaling techniques. First, we derive a closed form expression for the SU outage probability and an upper bound for the PU outage probability. Then, we optimize the SU signal parameters to minimize its outage probability while maintaining the required PU quality-of-service based on the average channel state information. Finally, we provide some numerical results that validate the tightness of the PU outage probability bound and demonstrate the advantage of employing the improper Gaussian signaling to the SU in order to access the spectrum of the FD PU.

Mohamed Gaafar, Osama Amin, Walid Abediseid and Mohamed-Slim Alouini
Computer, Electrical, and Mathematical Sciences and Engineering (CEMSE) Division King Abdullah University of Science and Technology (KAUST) Thuwal, Makkah Province, Saudi Arabia
e-mail: slim.alouini@kaust.edu.sa

IV-10

Energy Efficient Power Allocation for Cognitive MIMO Channels

Lokman Sboui, Zouheir Rezki, Ahmed Sultan and Mohamed-Slim Alouini

Due to the massive data traffic in wireless networks, energy consumption has become a crucial concern, especially with the limited power supply of the mobile terminals and the increasing CO2 emission of the cellular industry. In this context, we study the energy efficiency (EE) of MIMO spectrum sharing cognitive radio (CR) systems under power and interference constraints. We present an energy efficient power allocation framework based on maximizing the average EE per parallel channel resulting from the singular value decomposition (SVD) eigenmode transmission. We also present a sub-optimal low complex power allocation scheme based on the water-filling power allocation. In the numerical results, we show that the suboptimal power allocation achieves at least 95% of the optimal performance. In addition, we show that adopting more antennas is more energy efficient given the same power budget. Finally, we show that the interference threshold has a significant effect on both the EE and the SE only at high-power regime.

Lokman Sboui, Zouheir Rezki, Ahmed Sultan and Mohamed-Slim Alouini
Computer, Electrical, and Mathematical Sciences and Engineering (CEMSE) Division King Abdullah University of Science and Technology (KAUST) Thuwal, Makkah Province, Saudi Arabia
e-mail: {lokman.sboui, zouheir.rezki, ahmed.salem, slim.alouini}@kaust.edu.sa

IV-11

Simultaneous Wireless Information and Power Transfer for MIMO Amplify-and-Forward Relay

Fatma Benkhelifa, and Mohamed-Slim Alouini

In this paper, we investigate the simultaneous wireless information and power transfer (SWIPT) for the two-hop Multiple-Input Multiple-Output (MIMO) Amplify-and-Forward (AF) relay communication systems with the multi- antenna energy harvesting relay. We derive the optimal source and relay covariance matrices to characterize the achievable region between the source- destination rate and the harvested energy at the relay, namely Rate-Energy (R-E) region. In this context, we consider the ideal scenario where the energy harvester (EH) receiver and the information decoder (ID) receiver at the relay can simultaneously decode the information and harvest the energy at the re- lay. Then, we consider more practical schemes which are the power splitting (PS) and the time switching (TS) which separate the EH and ID transfer over the power domain and the time domain, respectively.

Fatma Benkhelifa, and Mohamed-Slim Alouini
Computer, Electrical, and Mathematical Sciences and Engineering (CEMSE) Division King Abdullah University of Science and Technology (KAUST) Thuwal, Makkah Province, Saudi Arabia
e-mail: {fatma.benkhelifa, slim.alouini}@kaust.edu.sa

Poster session V

Computational Electro-Magnetics

V-1

Efficient Computation of Electromagnetic Fields Scattered From Dielectric Objects of Uncertain Shapes Using a Multilevel Monte Carlo Scheme

Alexander Litvinenko, İsmail Enes Uysal, Hüseyin Arda Ülkü, Jesper Oppelstrup, Raúl Tempone, and Hakan Bağcı

Simulators capable of computing scattered fields from objects of uncertain shapes are highly useful in electromagnetics and photonics, where device designs are typically subject to fabrication tolerances. Knowledge of statistical variations in scattered fields is useful in ensuring error-free functioning of devices. Oftentimes such simulators use a Monte Carlo (MC) scheme to sample the random domain, where the variables parameterize the uncertainties in the geometry. At each sample, which corresponds to a realization of the geometry, a deterministic electromagnetic solver is executed to compute the scattered fields. However, to obtain accurate statistics of the scattered fields, the number of MC samples has to be large. This significantly increases the total execution time. In this work, to address this challenge, the Multilevel MC (MLMC [1]) scheme is used together with a (deterministic) surface integral equation solver. The MLMC achieves a higher efficiency by "balancing" the statistical errors due to sampling of the random domain and the numerical errors due to discretization of the geometry at each of these samples. Error balancing results in more (less) number of samples requiring coarser (finer) discretizations. Consequently, total execution time is significantly shortened. Numerical results demonstrating the efficiency of this proposed simulator are presented.

References

1. N. Collier, A.-L. Haji-Ali, F. Nobile, E. von Schwerin, R. Tempone, *A Continuation Multilevel Monte Carlo algorithm*, BIT Numerical Mathematics, 2014
2. C. Chauviere, J. D. Hesthaven, L. C. Wilcox, *Efficient computation of RCS from scatterers of uncertain shapes*, IEEE Transactions on Antennas and propagation, Vol. 55, N5, 2007
3. Zh. Zeng, J.-M. Jin, *Efficient calculation of scattering variation due to uncertain geometrical deviation*, Electromagnetics, 27:7387-398, 2007
4. D Liu, A Litvinenko, C Schillings, V Schulz, *Quantification of airfoil geometry-induced aerodynamic uncertainties-comparison of approaches*, arXiv preprint arXiv:1505.05731, 2015
5. A. Litvinenko, H. G. Matthies, *Numerical Methods for Uncertainty Quantification and Bayesian Update in Aerodynamics*, Chapter in the book - Management and Minimisation of Uncertainties and Errors in Numerical Aerodynamics, Vol. 122 of the series Notes on Numerical Fluid Mechanics and Multidisciplinary Design, pp 265-282, 2013, Springer
6. A. Litvinenko, H.G. Matthies, *Uncertainties quantification and data compression in numerical aerodynamics*, PAMM 11 (1), 877-878, 2011

Alexander Litvinenko, İsmail Enes Uysal, Hüseyin Arda Ülkü, Raúl Tempone, and Hakan Bağcı
Division of Computer, Electrical, and Mathematical Science and Engineering, King Abdullah University of Science and Technology , Thuwal, Saudi Arabia.
e-mail: {alexander.litvinenko,ismail.uysal,huseyin.ulku,raul.tempone,hakan.bagci}@kaust.edu.sa

J. Oppelstrup
NA/Mathematics KTH Kungl Tekniska Högskolan, Stockholm.
e-mail: jespero@nada.kth.se

V-2

Sparse Electromagnetic Imaging using Nonlinear Landweber Iterations

Abdulla Desmal and Hakan Bağcı

A scheme for efficiently solving the nonlinear electromagnetic inverse scattering problem on sparse investigation domains is described. The proposed scheme reconstructs the (complex) dielectric permittivity of an investigation domain from scattered fields measured away from the domain itself. Least-squares data misfit between the computed scattered fields, which are expressed as a nonlinear function of the permittivity, and the measured fields is constrained by the L_0/L_1-norm of the solution. The resulting minimization problem is solved using nonlinear Landweber iterations, where at each iteration a thresholding function is applied to enforce the sparseness-promoting L_0/L_1-norm constraint. The thresholded nonlinear Landweber iterations are applied to several two-dimensional problems, where the "measured" fields are synthetically generated or obtained from actual experiments. These numerical experiments demonstrate the accuracy, efficiency, and applicability of the proposed scheme in reconstructing sparse profiles with high permittivity values.

A. Desmal
Division of Electrical, Computer, and Mathematical Sciences and Engineering (CEMSE), King Abdullah University of Science and Technology (KAUST), Thuwal 23955-6900, Saudi Arabia.
e-mail: abdulla.desmal@kaust.edu.sa

H. Bağcı
Division of Electrical, Computer, and Mathematical Sciences and Engineering (CEMSE), King Abdullah University of Science and Technology (KAUST), Thuwal 23955-6900, Saudi Arabia.
e-mail: hakan.bagci@kaust.edu.sa

V-3

A Nonlinear Sparse Electromagnetic Imaging Scheme Accelerated with Projected Steepest Descent Algorithm

Abdulla Desmal and Hakan Bağcı

An efficient and accurate scheme for solving the nonlinear electromagnetic inverse scattering problem on three-dimensional (3D) sparse investigation domains is described. The proposed scheme achieves its efficiency and accuracy integrating two concepts: (i) The nonlinear optimization problem is constrained using the L_0/L_1 norm of the solution as the penalty term to alleviate the ill-posedness of the inverse problem. The resulting Tikhonov minimization problem is solved using thresholded nonlinear Landweber iterations. Thresholding promotes the sparseness in the solution resulting in sharper reconstructions/images. (ii) The efficiency of the Landweber iterations is significantly increased using a steepest descent algorithm equipped with a projection operator that is applied at every iteration together with the thresholding operation. Steepest descent algorithm ensures accelerated and convergent solution by utilizing larger iteration steps selected based on a necessary B-condition. Numerical experiments demonstrate the accuracy, efficiency, and applicability of the proposed method in reconstructing 3D sparse profiles.

A. Desmal
Division of Electrical, Computer, and Mathematical Sciences and Engineering (CEMSE), King Abdullah University of Science and Technology (KAUST), Thuwal 23955-6900, Saudi Arabia.
e-mail: abdulla.desmal@kaust.edu.sa

H. Bağcı
Division of Electrical, Computer, and Mathematical Sciences and Engineering (CEMSE), King Abdullah University of Science and Technology (KAUST), Thuwal 23955-6900, Saudi Arabia.
e-mail: hakan.bagci@kaust.edu.sa

V-4

A Sparsity-Regularized Reconstruction of Two-Dimensional Piecewise Continuous Domains

Ali Imran Sandhu, Abdulla Desmal, and Hakan Bağcı

Sparsity promoting regularization algorithms become inefficient in reconstructing investigation domains with piecewise continuous dielectric profiles. Piecewise continuity does not imply spatial sparseness in the investigation domain. To overcome this problem, a sparsity-regularized Born iterative method (BIM), which represents the electromagnetic scattered fields in terms of the spatial derivative of the dielectric profile and executes the minimization required for the reconstruction over the samples of the dielectric profile?s derivative, is proposed. Application of the derivative "sparsifies" the unknown to be reconstructed, increasing the efficiency of the sparsity-promoting regularization scheme. Then, like the traditional BIM, the nonlinear problem is linearized (in derivative samples) at each iteration and sparsity constraint is enforced on each linear problem using thresholded Landweber iterations. Numerical results demonstrate the efficiency and accuracy of the proposed scheme in reconstructing piecewise continuous profiles.

A. I. Sandhu
Division of Electrical, Computer, and Mathematical Sciences and Engineering (CEMSE), King Abdullah University of Science and Technology (KAUST), Thuwal 23955-6900, Saudi Arabia.
e-mail: aliimran.sandhu@kaust.edu.sa

A. Desmal
Division of Electrical, Computer, and Mathematical Sciences and Engineering (CEMSE), King Abdullah University of Science and Technology (KAUST), Thuwal 23955-6900, Saudi Arabia.
e-mail: abdulla.desmal@kaust.edu.sa

H. Bağcı
Division of Electrical, Computer, and Mathematical Sciences and Engineering (CEMSE), King Abdullah University of Science and Technology (KAUST), Thuwal 23955-6900, Saudi Arabia.
e-mail: hakan.bagci@kaust.edu.sa

V-5

Transient Analysis of Electromagnetic Wave interactions on Ferromagnetic Structures using Landau-Lifshitz-Gilbert and Volume Integral Equations

Sadeed Bin Sayed, Hüseyin Arda Ülkü, and Hakan Bağcı

Ferromagnetic materials are oftentimes used as substrates in reconfigurable microwave systems since their magnetization can be dynamically controlled using a biasing DC magnetic field. The nonlinear dependence of the magnetization on the fields induced inside a ferromagnetic material is governed by the Landau-Lifshitz-Gilbert (LLG) equation. In this work, a marching on in time (MOT) scheme for solving the coupled LLG and time domain volume integral (TDVI) equations expressed in unknowns magnetic field intensity and flux density. The proposed scheme discretizes the field and flux unknowns using half and full Schaubert-Wilton-Glisson (SWG) basis functions in space and polynomial temporal interpolators in time. The resulting coupled system of the discretized LLG and TDVI equations integrated in time using an explicit $PE(CE)^m$ scheme to yield the unknown expansion coefficients. Explicitness of time marching allows for incorporation of the nonlinearity as a simple function evaluation on the right/left hand sides of the coupled system of equations. Consequently, the resulting MOT scheme does not call for Newton-like nonlinear solvers. Numerical experiments demonstrate the applicability of the proposed MOT scheme to analyzing electromagnetic interactions on ferromagnetic scatterers.

S. B. Sayed
Division of Electrical, Computer, and Mathematical Sciences and Engineering (CEMSE), King Abdullah University of Science and Technology (KAUST), Thuwal 23955-6900, Saudi Arabia.
e-mail: sadeed.sayed@kaust.edu.sa

H. A. Ülkü
Division of Electrical, Computer, and Mathematical Sciences and Engineering (CEMSE), King Abdullah University of Science and Technology (KAUST), Thuwal 23955-6900, Saudi Arabia.
e-mail: huseyin.ulku@kaust.edu.sa
Electronics Engineering Department, Gebze Technical University, 41400 Gebze, Kocaeli, Turkey.
e-mail: haulku@gtu.edu.tr

H. Bağcı
Division of Electrical, Computer, and Mathematical Sciences and Engineering (CEMSE), King Abdullah University of Science and Technology (KAUST), Thuwal 23955-6900, Saudi Arabia.
e-mail: hakan.bagci@kaust.edu.sa

V-6

Analysis of Transient Electromagnetic Interactions on Nanodevices Using a Quantum-corrected Integral Equation Approach

İsmail Enes Uysal, Hüseyin Arda Ülkü, and Hakan Bağcı

Electromagnetic analysis of plasmonic nanostructures is traditionally carried out using numerical schemes that solve Maxwell equations supported with classical constitutive relations. However, quantum tunneling, i.e., electrons "jumping" between two structures that are separated from each other by a sub-nanometer gap, is not immediately accounted for by these classical numerical schemes. In this work, an auxiliary tunnel made of Drude material is used to "connect" these two structures and create support for the current generated by tunneled electrons (R. Esteban et al., *Nat. Commun.*, 3(825), 2012). The electromagnetic fields on the resulting connected structure are analyzed using a time domain surface integral equation solver. Time domain samples of the dispersive medium Green function and dielectric permittivity are computed from the analytical inverse Fourier transform applied to the rational function representation of their frequency domain samples.

İ. E. Uysal
Division of Electrical, Computer, and Mathematical Sciences and Engineering (CEMSE), King Abdullah University of Science and Technology (KAUST), Thuwal 23955-6900, Saudi Arabia.
e-mail: ismail.uysal@kaust.edu.sa

H. A. Ülkü
Division of Electrical, Computer, and Mathematical Sciences and Engineering (CEMSE), King Abdullah University of Science and Technology (KAUST), Thuwal 23955-6900, Saudi Arabia.
e-mail: huseyin.ulku@kaust.edu.sa
Electronics Engineering Department, Gebze Technical University, 41400 Gebze, Kocaeli, Turkey.
e-mail: haulku@gtu.edu.tr

H. Bağcı
Division of Electrical, Computer, and Mathematical Sciences and Engineering (CEMSE), King Abdullah University of Science and Technology (KAUST), Thuwal 23955-6900, Saudi Arabia.
e-mail: hakan.bagci@kaust.edu.sa

V-7

An Adaptive Hierarchical Sparse Grid Collocation Method for Stochastic Characterization of Electromagnetic/Circuit Systems

Ping Li, Lijun Jiang, and Hakan Bağcı

The adaptive hierarchical sparse grid collocation (ASGC) scheme is used together with the discontinuous Galerkin time-domain (DGTD) method to quantify the effects of uncertain device parameters on the response of integrated electromagnetic/circuit systems. The ASGC scheme approximates the random variables of interest using interpolation functions defined over a set of collocation points. The weights and locations of these points are determined by the well-known Smolyak's algorithm utilizing an adaptive refinement strategy. This improved sampling technique calls for more points along the dimensions with sharp variations and/or discontinuities and less points along those with smooth variations, resulting in a non-uniform distribution of points and consequently reduces the computation time for a given level of accuracy. The "function" evaluations, which are required by the ASGC scheme at the collocation points (i.e., a given set of parameters of the electromagnetic/circuit system) are carried out by the DGTD method.

P. Li
Division of Electrical, Computer, and Mathematical Sciences and Engineering (CEMSE), King Abdullah University of Science and Technology (KAUST), Thuwal 23955-6900, Saudi Arabia.
e-mail: ping.li@kaust.edu.sa

L. Jiang
Department of Electrical and Electronics Engineering, University of Hong Kong, Hong Kong.
e-mail: jianglj@hku.hk

H. Bağcı
Division of Electrical, Computer, and Mathematical Sciences and Engineering (CEMSE), King Abdullah University of Science and Technology (KAUST), Thuwal 23955-6900, Saudi Arabia.
e-mail: hakan.bagci@kaust.edu.sa

Poster session VI

Reactive Computational Fluid Dynamics

VI-1

New Bayesian inference method using two steps of Markov chain Monte Carlo and its application to shock tube experimental data of Furan oxidation

Daesang Kim, Iman E. Gharamti, Fabrizio Bisetti, Ahmed Elwardani, Aamir Farooq, and Omar M. Knio

A new Bayesian inference method has been developed and applied to Furan shock tube experimental data for efficient statistical inferences of the Arrhenius parameters of two OH radical consumption reactions. The collected experimental data, which consist of time series signals of OH radical concentrations of 14 shock tube experiments, may require several days for MCMC computations even with the support of a fast surrogate of the combustion simulation model, while the new method reduces it to several hours by splitting the process into two steps of MCMC: the first inference of rate constants and the second inference of the Arrhenius parameters. Each step has low dimensional parameter spaces and the second step does not need the executions of the combustion simulation. Furthermore, the new approach has more flexibility in choosing the ranges of the inference parameters, and the higher speed and flexibility of the method enable the more accurate inferences and the analyses of the propagation of errors in the measured temperatures and the alignment of the experimental time to the inference results.

Daesang Kim, Iman E. Gharamti, Fabrizio Bisetti, Ahmed Elwardani, Aamir Farooq, and Omar M. Knio
Computer, Electrical and Mathematical Sciences & Engineering Division King Abdullah University of Science and Technology (KAUST), Saudi Arabia

VI-2

Optimal design of experiments considering noisy control parameters for the inference of Furan combustion reaction rate

Quan Long, Daesang Kim, Fabrizio Bisetti, Aamir Farooq, Raúl F. Tempone and Omar M. Knio

We carry out the design of experiments for the identification of the reaction parameters in Furan combustion. The lacks of information on the true value of the control parameters, specifically, the initial temperature and the initial TBHP concentration, are considered in the design procedure by errors-invariables models. We use two types of observables. The first is a scaler observable, i.e., half decay time of the [TBHP]. The second is the time history of the concentration.

Quan Long
United Technologies Research Center, East Hartford, CT, USA
e-mail: longq@utrc.utc.com

Daesang Kim, Fabrizio Bisetti and Aamir Farooq
Clean Combustion Research Center, KAUST, KSA
e-mail: daesang.kim@kaust.edu.sa, fabrizio.bisetti@kaust.edu.sa, aamir.farooq@kaust.edu.sa

Raúl Tempone and Omar M. Knio

Computer, Electrical and Mathematical Sciences & Engineering Division King Abdullah University of Science and Technology (KAUST), Saudi Arabia
e-mail: raul.tempone@kaust.edu.sa, omar.knio@kaust.edu.sa

Poster session VII

Other Applications

VII-1

A mathematical model of Delamination in Composite Materials

Ben Mansour Dia, Luis Espath, Lakhsmi Selvakumaran, Serge Prudhomme and Raúl Tempone

A mathematical model of delamination crack along a thin interface layer is presented. This work combines theoretical and numerical study that has been conducted on the delamination of fibre reinforced polymeric composites. The composite laminate that will be used in the Benmarck problem have the configuration [0/90/0] with each layer having a thickness of $1mm$. Numerical results, based on the finite elements method with Lagrange multipliers, are presented for the forward problem.

Ben Mansour Dia, Luis Espath, Lakhsmi and Raúl Tempone
Computer, Electrical, and Mathematical Sciences and Engineering (CEMSE) Division King Abdullah University of Science and Technology (KAUST), Saudi Arabia e-mail: {benmansour.dia,luis.espath,raul.tempone}@kaust.edu.sa

Lakhsmi Selvakumaran
Physical Science and Engineering (PSE) Division King Abdullah University of Science and Technology (KAUST), Saudi Arabia

Serge Prudhomme
Department of Mathematical and Industrial Engineering, Ecole Polytechnique Montréal, Canada.

VII-2

Generalized Chebyshev Nodes and Application to RBF Approximation

Sören Wolfers

Scattered data approximation encompasses a set of techniques used to reconstruct functions from unstructured data. Of these techniques, one of the most frequently utilized is interpolation by radial basis functions (RBF). While RBF have been successfully applied to multidimensional interpolation and the numerical solution of partial differential equations, approximation quality decreases near the boundary of the domain unless more interpolation nodes are placed nearby. The goals of this work are twofold. The first is to provide a general framework for clustering nodes near the boundary in general domains. We propose node sets that behave much like the univariate Chebyshev nodes and we bound their associated Lebesgue constants for generalized polynomial interpolation. These bounds are used to derive new sampling inequalities for RBF interpolation. We additionally provide results on meshless collocation of boundary value problems. We argue that collocation nodes should have the same density on the boundary and within the domain.

References:

1. Wolfers, S. (2015), Boundary effects in scattered data approximation. Master's thesis, University of Bonn.

Sören Wolfers
Division of Computer, Electrical and Mathematical Sciences &Engineering, King Abdullah University of Science and Technology, Saudi Arabia.
e-mail: soeren.wolfers@kaust.edu.sa

VII-3

Tight Error Bounds for Fourier methods for option pricing for exponential Lévy processes

Fabián Crocce, Juho Häppölä, Jonas Kiessling and Raúl Tempone

Lévy processes form a wide range of models for describing the dynamics of financial asset prices. Financial derivatives written on Lévy driven assets can be priced using partial integro-differential equations, (PIDEs). Thanks to the Lévy-Khintchine formula, these Lévy processes have an explicit frequency space representation. This representation gives access to the computationally efficient FFT methods allowing not only spectral convergence of derivative prices, but also the simultaneous evaluation of the value function at a mesh of multiple points. We represent the numerical treatment and error analysis of FFT methods in derivative pricing when underlying asset is modelled by an exponential Lévy process.

Fabián Crocce, Juho Häppölä and Raúl Tempone
King Abdullah University of Science and Technology, Thuwal, Kingdom of Saudi Arabia
e-mail: fabian.crocce,

Jonas Kiessling
NA/Mathematics KTH Kungl Tekniska Högskolan, Stockholm.
e-mail: ...@kth.se

VII-4

Basket call option pricing for CCVG using sparse grids

Fabián Crocce, Juho Häppölä, Alessandro Iania and Raúl Tempone

Common clock variance gamma has been considered in the literature to model prices of a set of correlated assets. We propose an algorithms to compute option prices under this model. We depart from the fundamental theorem of option pricing, which states that the price of a derivative is the expected income under a specific measure called risk-neutral. Our algorithm compute this expected income by computing the corresponding multidimensional integral using sparse grids to overcome the course of dimensionality.

Fabián Crocce, Juho Häppölä, Alessandro Iania and Raul Tempone
King Abdullah University of Science and Technology, Thuwal, Kingdom of Saudi Arabia

VII-5

Some Numerical Aspects on Crowd Motion - The Hughes' Model

Diogo A. Gomes and Roberto M. Velho

Here, we study a crowd model proposed by Roger Hughes in [1] and describe a numerical approach to solve it. This model comprises a Fokker-Planck equation coupled with an Eikonal in a 2-dimensional domain Ω with Dirichlet or Neumann data:

$$\begin{cases} \rho_t(x,t) + \div(\rho(1-\rho)^2 Du) = \Delta\rho, \\ |Du(x)|^2 = \dfrac{1}{(1-\rho)^2}. \end{cases} \tag{VII-5.1}$$

The Fokker-Planck equation gives the evolution of the crowd density ρ. The Eikonal equation determines the optimal direction of movement for each individual if the rest of the population remains frozen.

We study periodic and Dirichlet/Neumann boundary conditions and special cases such as stationary and radial solutions. Open topics include qualitative properties of this system, for example, the decay of L^p norms in time or special solutions, and a qualitative description of its dynamics. Although significant progress has been achieved in [2], even 1-dimensional models are not completely understood.

We propose a numerical method that explores the adjoint structure present in this system, and we compare it to classical schemes of discretization - for 1-D models. One feature of our method is the conservation of the mass of agents.

These models can give important clues to the optimal design of routes. For example, answering the question on whether adding barriers at specific places can help the traffic of people assists in determining the ideal number of exits and their size - ensuring a given evacuation time. Variations in this model include agents with different mobilities and nonlinearities [3].

References:

[1] R. L. Hughes *A continuum theory for the flow of pedestrians* - 2002: Journal of Differential Equations - Transportation Research Part B - 507-535.

[2] M. Di Francesco, P. Markowich, J.-F. Pietschmann and M.-T. Wolfram *On the Hughes' model for pedestrian flow: the one-dimensional case* - 2011: Journal of Differential Equations - Vol. 250 - 1334-1362.

[3] M. Burger, M. Di Francesco, P. Markowich and M.-T. Wolfram *Mean field games with nonlinear mobilities in pedestrian dynamics* - 2013.

Diogo A. Gomes and Roberto M. Velho
King Abdullah University of Science and Technology, Thuwal, Kingdom of Saudi Arabia
e-mail: roberto.velho@gmail.com

VII-6

Computable error estimation for FEM for elliptic PDE with lognormal data

Eric Hall

We derive computable error estimates for finite element approximations to elliptic PDE with rough, stochastic coefficients. In particular, we consider problems arising in subsurface flow where the coefficients are assumed to have a lognormal distribution. These estimators, based on local error indicators, are for observables of the pathwise Galerkin errors and of the expected quadrature errors committed in piecewise linear finite element approximations. Our theory is supported by numerical experiments for test problems in one and two dimensions.

Eric Hall
Department of Mathematics & Statistics, University of Massachusetts.
e-mail: hall@math.umass.edu

VII-7

Overview of robust optimal problems for random PDEs using different risk measures

Fabio Nobile and Mathieu Martin

We present an overview of formulations of optimal control problems for systems governed by PDEs with uncertain coefficients using different risk measures for the functional to be minimized. We will review the main well posedness results for the optimal control problem, in the case of a general convex risk measure and consider a Monte Carlo approximation combined with a steepest descent algorithm.

Fabio Nobile and Mathieu Martin
SB-MATHICSE-CSQI, EPFL, Lausanne, Switzerland
e-mail: matthieu.martin@epfl.ch

VII-8

A new smoothing technique for basket options

Markus Siebenmorgen, Christian Bayer, Raúl Tempone

The computation of the price of European basket options in a Black-Scholes model leads in certain cases to the calculation of the integral

$$E\left[\left(\sum_{i=1}^{d} w_i e^{X_i} - K\right)^+\right], \tag{VII-8.1}$$

where X follows $\mathcal{N}(0,\Sigma)$ with a covariance matrix Σ and $d >> 1$. Hence, we have to compute the integral of an integrand with a kink over the integration domain $\mathbb{R}^d$. We provide a simple method for smoothing the integrand which produces an analytic integrand and is able to reduce the dimensionality of the integration problem by (1). In particular, we transform the (d)-dimensional random variable in such a way that it is feasible to apply the famous Black-Scholes formula with respect to a single coordinate. The resulting integration problem over $\mathbb{R}^{d-1}$ with an analytic integrand is then solved by an adaptive sparse grid approach. This leads, at least in considerably high dimensions, to better convergence results compared to those of standard Monte Carlo or quasi-Monte Carlo quadratures.

Markus Siebenmorgen at Institute for Numerical Simulation, University of Bonn, Germany
e-mail: markus.siebenmorgen@unibas.ch

Christian Bayer
Weierstrass Institute for Applied Analysis and Stochastics, Berlin
e-mail: christian.bayer@wias-berlin.de

Raúl Tempone
at Computer, Electrical and Mathematical Sciences & Engineering Division King Abdullah University of Science and Technology (KAUST), Saudi Arabia

VII-9

Optimization under Uncertainty

Rafael Holdorf Lopez

The goal of this poster is to present the main approaches to optimization of engineering systems in the presence of uncertainties. First, the basic concepts of optimization and uncertainty quantification are presented separately. Then, the optimization under uncertainties techniques are described. We begin by giving an insight about robust optimization. Next, we detail how to deal with probabilistic constraints in optimization, the so called the reliability based design. Subsequently, we present the risk optimization approach, which includes the expected costs of failure in the objective function. Finally, potential topics of research in these areas are pointed out.

Rafael Holdorf Lopez
Department of Civil Engineering at the Federal University of Santa Catarina, Brazil.
e-mail: rafaelholdorf@gmail.com

VII-10

A Stochastic Multiscale Method for the Elastic Wave Equations Arising from Fiber Composites

Ivo Babuska and Mohammad Motamed and Raúl Tempone

We present a stochastic multilevel global-local algorithm for computing elastic waves propagating in fiber-reinforced polymer composites, where the material properties and the size and distribution of fibers in the poly- mer matrix may be random. The method aims at approximating statistical moments of some given quantities of interest, such as stresses, in regions of relatively small size, e.g. hot spots or zones that are deemed vulnerable to failure. For a fiber-reinforced cross-plied laminate, we introduce three problems: 1) macro; 2) meso; and 3) micro problems, corresponding to the three natural length scales: 1) the sizes of plate; 2) the tickles of plies; and 3) and the diameter of fibers. The algorithm uses a homogenized global solution to construct a local approximation that captures the microscale features of the problem. We perform numerical experiments to show the applicability and efficiency of the method.

Ivo Babuska
The Institute for Computational Engineering and Sciences, The University of Texas at Austin, USA
e-mail: babuska@ices.texas.edu

Mohammad Motamet
Department of Mathematics and Statistics, The University of New Mexico, USA
e-mail: motamed@math.unm.edu

Raúl Tempone
Computer, Electrical and Mathematical Sciences & Engineering Division, KAUST, Saudi Arabia
e-mail: raul.tempone@kaust.edu.sa

VII-11

Computation of High-Frequency Waves with Random Uncertainty

Gabriela Malenova, Mohammad Motamed, Olof Runborg and Raúl Tempone

We consider the forward propagation of uncertainty in high-frequency waves, described by the second order wave equation with highly oscillatory initial data. The main sources of uncertainty are the wave speed and/or the initial phase and amplitude, described by a finite number of random variables with known joint probability distribution. We propose a stochastic spectral asymptotic method for computing the statistics of uncertain output quantities of interest (QoIs), which are often linear or non- linear functionals of the wave solution and its spatial/temporal derivatives. The numerical scheme combines two techniques:

- a high-frequency method based on Gaussian beams,
- a sparse stochastic collocation method.

The fast spectral convergence of the proposed method depends crucially on the presence of high stochastic regularity of the QoI independent of the wave frequency. In general, the high-frequency wave solutions to para- metric hyperbolic equations are highly oscillatory and non-smooth in both physical and stochastic spaces. Consequently, the stochastic regularity of the QoI, which is a functional of the wave solution, may in principle be low and depend on frequency. In the present work, we provide theoretical arguments and numerical evidence that physically motivated QoIs based on local averages of $|u^\varepsilon|^2$ are smooth, with derivatives in the stochastic space uniformly bounded in ε, where $u\varepsilon$ and ε denote the highly oscillatory wave solution and the short wavelength, respectively. This observable related regularity makes the proposed approach more efficient than current asymptotic approaches based on Monte Carlo sampling techniques.

Gabriela Malenova and Olof Runborg
Department of Mathematics, KTH Royal Institute of Technology, Sweden
e-mail: malenova@kth.se, olofr@kth.se

Mohammad Motamet
Department of Mathematics and Statistics, The University of New Mexico, USA
e-mail: motamed@math.unm.edu

Raúl Tempone
Computer, Electrical and Mathematical Sciences & Engineering Division, KAUST, Saudi Arabia
e-mail: raul.tempone@kaust.edu.sa

VII-12

Flow, transport and diffusion in random geometries II: applications

Pietro Asinari, Diego Ceglia, Matteo Icardi, Serge Prudhomme and Raúl Tempone

Multilevel Monte Carlo (MLMC) is an efficient and flexible solution for the propagation of uncertainties in complex models, where an explicit parametrization of the input randomness is not available or too expensive. We present several applications of our MLMC algorithm for flow, transport and diffusion in random heterogeneous materials. The absolute permeability and effective diffusivity (or formation factor) of micro-scale porous media samples are computed and the uncertainty related to the sampling procedures is studied. The algorithm is then extended to the transport problems and multiphase flows for the estimation of dispersion and relative permeability curves. The impact of water drops on random stuctured surfaces, with microfluidics applications to self-cleaning materials, is also studied and simulated. Finally the estimation of new drag correlation laws for poly-dispersed dilute and dense suspensions is presented.

Pietro Asinari and Diego Ceglia
Dipartimento di Energia, Politecnico di Torino, Italy.
e-mail: pietro.asinari@polito.it,diego.ceglia@kaust.edu.sa

Matteo Icardi and Raúl Tempone
Computer, Electrical and Mathematical Sciences & Engineering Division, KAUST, Saudi Arabia
e-mail: matteo.icardi@kaust.edu.sa, raul.tempone@kaust.edu.sa

Serge Prudhomme
Department of Mathematics and Industrial Engineering, Ecole Polytechnique de Montréal, Montréal, Canada
e-mail: serge.prudhomme@polymtl.ca

VII-13

Flow in Random Microstructures: a Multilevel Monte Carlo Approach

Matteo Icardi and Raúl Tempone

In this work we are interested in the fast estimation of effective parameters of random heterogeneous materials using Multilevel Monte Carlo (MLMC). MLMC is an efficient and flexible solution for the propagation of un- certainties in complex models, where an explicit parametrisation of the input randomness is not available or too expensive. We propose a general-purpose algorithm and computational code for the solution of Partial Differential Equations (PDEs) on random heterogeneous materials. We make use of the key idea of MLMC, based on different discretisation levels, extending it in a more general context, making use of a hierarchy of physical resolution scales, solvers, mod- els and other numerical/geometrical discretisation parameters. Modifications of the classical MLMC estimators are proposed to further reduce variance in cases where analytical convergence rates and asymptotic regimes are not avail- able. Spheres, ellipsoids and general convex-shaped grains are placed randomly in the domain with different placing/packing algorithms and the effective properties of the heterogeneous medium are computed. These are, for example, effective diffusivities, conductivities, and reaction rates. The implementation of the Monte-Carlo estimators, the statistical samples and each single solver is done efficiently in parallel. The method is tested and applied for pore-scale simulations of random sphere packings.

Matteo Icardi
Mathematics Institute, University of Warwick.
e-mail: matteo.icardi@warwick.ac.uk

Raúl Tempone
Computer, Electrical and Mathematical Sciences & Engineering Division, KAUST, Saudi Arabia
e-mail: raul.tempone@kaust.edu.sa

This booklet has been edited by Ben Mansour Dia, Alexander Litvinenko and many other people from SRI UQ Center. Please contact benmansour.dia@kaust.edu.sa or alexander.litvinenko@kaust.edu.sa for any questions regarding this booklet.