WIAS/GAMM/TUM Summer School on Uncertainty Quantification 2016

Weierstrass Institute for Applied Analysis and Stochastics
September 12 – 16, 2016

www.wias-berlin.de/workshops/uq-school16/

Weierstraß-Institut für
Angewandte Analysis und Stochastik

www.wias-berlin.de

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Contents

Welcome

Dear participant of the Uncertainty Quantification Summer School,

welcome to the Weierstrass Institute for Applied Analysis and Stochastics (WIAS) in Berlin. Our Uncertainty Quantification Summer School is jointly organized by the GAMM Activity Group on Uncertainty Quantification, the International Research and Training (IGDK1754) Group Munich-Graz and WIAS. We gratefully acknowledge financial support by the IGDK1754, WIAS and the Einstein Center for Mathematics Berlin (ECMath).

Given below is some general information regarding logistics and other arrangements for our summer school.

Entry into the building requires displaying your participant's badge to the receptionist at the entrance desk. Please wear your badge, as the receptionist is not supposed to let you in without it.

Lunch can be taken in a number of restaurants and snack bars in the neighbourhood of the institute, see an extra sheet for more details.

The Conference Dinner will be held in the restaurant *UMSPANNWERK Ost*, Palisadenstr. 48, 10243 Berlin, on Monday, September 12, 2016 at 20.00 p.m.

Smoking in the building is not allowed.

We wish you a pleasant week and a stimulating learning experience.

Kind regards,

Alexey Chernov,
Martin Eigel,
Oliver Ernst,
Michael Hintermüller,
Reinhold Schneider,
Elisabeth Ullmann
(Organizers)

Monday, September 12, 2016

07:30	Registration
08:20	Opening Remarks
08:30	**Raúl Tempone** Lecture 1: On Monte Carlo, Multilevel Monte Carlo and Adaptive Multilevel Monte Carlo
10:00 – 10:30	Coffee
10:30	**Raúl Tempone** Lecture 2: Multi-index Monte Carlo and Multi-index Stochastic Collocation
12:00 – 14:00	Lunch
14:00	**Raúl Tempone** Lab Session
16:30 – 19:30	Walking tour in Berlin
20:00	Dinner

Tuesday, September 13, 2016

08:30	**Bruno Sudret** Lecture 1: Sparse Polynomial Expansions for Uncertainty Propagation and Sensitivity Analysis
10:00 – 10:30	Coffee
10:30	**Bruno Sudret** Lecture 2: Structural Reliability Methods for Engineering Risk Analysis
12:00 – 14:00	Lunch
14:00	**Bruno Sudret** Lab Session
16:00 – 16:30	Coffee
17:00	Public lecture: **Gerd Gigerenzer** Center for Adaptive Behaviour and Cognition Max-Planck Institute for Human Development, Berlin **Homo Heuristicus: Heuristic Decision Making**

Wednesday, September 14, 2016

08:30	**Lars Grasedyck** Lecture 1: Hierarchical Low Rank Tensor Formats
10:00 – 10:30	Coffee
10:30	**Lars Grasedyck** Lecture 2: Low Rank Model Reduction and Uncertainty Quantification
12:00 – 14:00	Lunch
14:00	**Lars Grasedyck/Christian Löbbert** Lab Session
16:00 – 16:30	Coffee
16:30 – 18:30	spare time/informal discussions

Thursday, September 15, 2016

08:30	**Claudia Schillings** Lecture 1: Introduction to the Bayesian Approach to Inverse Problems
10:00 – 10:30	Coffee
10:30	**Claudia Schillings** Lecture 2: Introduction to the Bayesian Approach to Inverse Problems
12:00 – 14:00	Lunch
14:00	**Claudia Schillings** Lab Session
16:00 – 16:30	Coffee
16:30 – 18:30	spare time/informal discussions

Friday, September 16, 2016

08:30	**Howard Elman** Lecture 1: Reduced-Order Models for Parameter-Dependent Partial Differential Equations
10:00 – 10:30	Coffee
10:30	**Howard Elman** Lecture 2: Reduced-Order Models for Parameter-Dependent Partial Differential Equations
12:00 – 14:00	Lunch
14:00	**Howard Elman** Lab Session
16:00 – 16:30	Coffee

Howard Elman (University of Maryland)

Reduced-Order Models for Parameter-Dependent Partial Differential Equations

We are interested in the efficient numerical solution of parameterized partial differential equations (PDEs) $\mathcal{L}_{\boldsymbol{\xi}} u(\cdot, \boldsymbol{\xi}) = f$ on a spatial domain $\mathcal{D}$, where the differential operator $\mathcal{L}$ depends on (a vector of) m parameters $\boldsymbol{\xi} \equiv (\xi_1, \ldots, \xi_m)^T$. A simple example is the diffusion operator $\mathcal{L}_{\boldsymbol{\xi}} = -\nabla a(\cdot, \boldsymbol{\xi})\nabla$ where the diffusion coefficient is a random field, i.e., for each $x \in \mathcal{D}$, $a(x, \cdot)$ is a random variable depending on $\boldsymbol{\xi}$; other scenarios, for example with parameterized boundary conditions, wave numbers in acoustics or convection terms, are also possible. For any given $\boldsymbol{\xi}$, discretization of the PDE in space leads to a finite-dimensional algebraic system of equations $F_{\boldsymbol{\xi}}(\mathbf{u}_{\boldsymbol{\xi}}) = 0$ whose solution (which gives a discrete approximation $u_h(\cdot, \boldsymbol{\xi})$ to the PDE solution) also depends on $\boldsymbol{\xi}$. If high-resolution accuracy is desired, then the solution of the discrete models tends to be costly, and if in addition solutions are required for many parameters, then costs become prohibitive. We will discuss the use of *reduced-order models* based on *reduced-basis methods* to reduce these costs.

Let N denote the size (number of degrees of freedom) of the discrete system $F_{\boldsymbol{\xi}}(\mathbf{u}_{\boldsymbol{\xi}}) = 0$. The idea behind reduced-basis methods is to compute solutions $\mathbf{u}_{\boldsymbol{\xi}_1}, \ldots, \mathbf{u}_{\boldsymbol{\xi}_n}$ of this system corresponding to a specific set of parameters $\{\boldsymbol{\xi}^{(1)}, \ldots, \boldsymbol{\xi}^{(n)}\}$, where $n \ll N$, and then, for other choices of $\boldsymbol{\xi}$, to compute approximate (or *surrogate*) solutions $\mathbf{u}_{\boldsymbol{\xi}}^{(s)}$ from the space spanned by the set of so-called "snapshot solutions" $\{\mathbf{u}_{\boldsymbol{\xi}_j}\}_{j=1}^n$. If Q is a matrix whose columns span the space of snapshot solutions, then the surrogate solution associated with parameter $\boldsymbol{\xi}$ has the form $\mathbf{u}_{\boldsymbol{\xi}}^{(s)} = Q\mathbf{y}_{\boldsymbol{\xi}}$. A typical strategy used to define the reduced problem is to impose a Galerkin condition, i.e., to require $Q^T F_{\boldsymbol{\xi}}(Q\mathbf{y}_{\boldsymbol{\xi}}) = 0$, so that the residual of the surrogate solution is orthogonal to the space spanned by the snapshots.

Two important aspects of this methodology are that the reduced solution should be an accurate approximation of the original (full) discrete system, and that the reduced problem should be much less expensive to solve. We will discuss various issues that enable these conditions to be valid as well as some things that are not fully resolved. Topics to be discussed include

- The separation of "offline" computations required to find the snapshot solutions and "online" computations used to find the surrogate solutions for multiple parameters.
- The costs of performing the online computations and the impact on the size of the parameter set on efficiency in the case of linear models.
- Issues that arise when the dependence of the model on the parameters is nonlinear, and ways to avoid some of the pitfalls that arise in this case.

Lars Grasedyck (RWTH Aachen)

Low-Rank Tensor Approximation

Lecture 1: Hierarchical Low Rank Tensor Formats

The first lecture on hierarchical low rank formats starts with a general introduction to notions of rank in higher dimensions, namely Canonical Polyadic (CP), Tucker, TT and Hierarchical Tucker (HT) ranks and the corresponding data-sparse tensor representations. Each of the notions of rank gives rise to a different set or manifold of tensors of fixed rank and we compare the advantages and drawbacks between the different formats. The concepts are introduced in the discrete setting where a tensor is a mapping from a d-fold Cartesian product of finite index sets, but we also point out the relation to d-variate functions, the continuous setting. We summarize some interesting open questions that open new and sometimes very difficult areas of research.

Lecture 2: Low Rank Model Reduction and Uncertainty Quantification

The second lecture is devoted to the application of hierarchical low rank formats for uncertainty quantification, or more specifically for the data-sparse representation of parameter dependent quantities of interest. The data-sparse low rank formats have a strong relation to reduced basis techniques for linear and nonlinear model reduction, but both methods have their individual advantages or disadvantages. The most challenging question in this area is whether or not the object of interest possesses the low rank structure and how one can reliably approximate it. From the data sparse low rank representation of the object of interest one can quickly but not trivially derive a variety of interesting quantities like expectation, variance, correlations etc.

Claudia Schillings (University Warwick)

Introduction to the Bayesian Approach to Inverse Problems

Uncertainty quantification (UQ) is an interesting, fast growing research area aiming at developing methods to address, characterize and minimize the impact of parameter, data and model uncertainty in complex systems. Applications of uncertainty quantification include all areas of engineering, environmental, physical and biological systems, e.g., groundwater flow problems, shape uncertainties in aerodynamic applications or nano-optics, biochemical networks and finance. The efficient treatment of uncertainties in mathematical models requires ideas and tools from various disciplines including numerical analysis, statistics, probability and computational science. In this course, we will focus on the identification of parameters through observations of the response of the system - the inverse problem. The uncertainty in the solution of the inverse problem will be described via the Bayesian approach. We will derive Bayes' theorem in the infinite dimensional setting and discuss properties such as well-posedness, statistical estimates and connections to classical regularization methods. The second part of this course will be devoted to algorithms for the efficient approximation of the solution of the Bayesian inverse problem.

Raúl Tempone (King Abdullah University of Science and Technology (KAUST))

Multilevel and Multiindex Monte-Carlo Methods

Lecture 1: On Monte Carlo, Multilevel Monte Carlo and Adaptive Multilevel Monte Carlo

We will first recall, for a general audience, the use of Monte Carlo and Multi-level Monte Carlo methods in the context of Uncertainty Quantification. Then we will discuss the recently developed Adaptive Multilevel Monte Carlo (MLMC) Methods for (i) Itŏ Stochastic Differential Equations, (ii) Stochastic Reaction Networks modeled by Pure Jump Markov Processes and (iii) Partial Differential Equations with random inputs. In this context, the notion of adaptivity includes several aspects such as mesh refinements based on either a priori or a posteriori error estimates, the local choice of different time stepping methods and the selection of the total number of levels and the number of samples at different levels. Our Adaptive MLMC estimator uses a hierarchy of adaptively refined, non-uniform time discretizations, and, as such, it may be considered a generalization of the uniform discretization MLMC method introduced independently by M. Giles and S. Heinrich. In particular, we show that our adaptive MLMC algorithms are asymptotically accurate and have the correct complexity with an improved control of the multiplicative constant factor in the asymptotic analysis. In this context, we developed novel techniques for estimation of parameters needed in our MLMC algorithms, such as the variance of the difference between consecutive approximations. These techniques take particular care of the deepest levels, where for efficiency reasons only few realizations are available to produce essential estimates. Moreover, we show the asymptotic normality of the statistical error in the MLMC estimator, justifying in this way our error estimate that allows prescribing both the required accuracy and confidence level in the final result. We present several examples to illustrate the above results and the corresponding computational savings.

References

1. A Continuation Multilevel Monte Carlo algorithm, by N. Collier, A.-L. Haji-Ali, F. Nobile, E. von Schwerin and R. Tempone. BIT Numer. Math., 55, pp. 399–432, 2015.

2. Optimization of mesh hierarchies in Multilevel Monte Carlo samplers of SDEs and PDEs with stochastic coefficients, by A.-L. Haji-Ali, F. Nobile, E. von Schwerin and R. Tempone. Stochastic Partial Differential Equations: Analysis and Computations, Vol. 4, Issue 1, Pages 76–112, 2016.

3. Implementation and Analysis of an Adaptive Multi-Level Monte Carlo Algorithm, by H. Hoel, E. von Schwerin, A. Szepessy, and R. Tempone. Monte Carlo Methods and Applications, 20(1), pp. 1–41, 2014.

4. Multilevel Hybrid Chernoff Tau-leap, by A. Moraes, R. Tempone and P. Vilanova. BIT Numerical Mathematics, Volume 56, Issue 1, pp. 189–239, 2016.

5. A multilevel adaptive reaction-splitting simulation method for stochastic reaction networks, by A. Moraes, R. Tempone and P. Vilanova. arXiv:1406.1989v1. To appear in SIAM Journal on Scientific Computing (SISC), 2016.

6. Multi-level drift-implicit tau-leap, by C. Ben Hammouda, A. Moraes and R. Tempone. arXiv:1512.00721. To appear in the Journal of Numerical Algorithms, 2016.

Lecture 2: Multi-index Monte Carlo and Multi-index Stochastic Collocation

We describe and analyze the Multi-Index Monte Carlo (MIMC) and the Multi-Index Stochastic Collocation method (MISC) for computing statistics of the solution of a PDE with random data. MIMC 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. These mixed differences yield 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. 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 efficient. We finally show the effectiveness of MIMC and MISC in some computational tests, including PDEs with random coefficients and Stochastic Particle Systems.

References

1. Multi-Index Stochastic Collocation for random PDEs, by A. L. Haji Ali, F. Nobile, L. Tamellini and R. Tempone. To appear in Computers and Mathematics with Applications, 2016.

2. Multi-index Stochastic Collocation convergence rates for random PDEs with parametric regularity, by A. Haji-Ali, F. Nobile, L. Tamellini, R. Tempone, Computers and Mathematics with Applications, Vol. 306, pp. 95-122, 2016.

3. Multi Index Monte Carlo: When Sparsity Meets Sampling, by A.-L. Haji-Ali, F. Nobile, and R. Tempone. Numerische Mathematik, Vol. 132(4), pp. 767–806, 2016.

Bruno Sudret (ETH Zurich)

Uncertainty Quantification in Engineering Risk Analysis

Uncertainty quantification (UQ) has become an important topic in engineering sciences in order to design robust and safe structures and systems. The key point for applications is that simulation models for assessing the systems' performance preexist before UQ is considered. Moreover, those models tend to be of increasing fidelity with respect to reality, meaning that the computational power requested for each single simulation is large, even when using cluster facilities. In practice, time and cost constraints of industrial projects allow the engineers to run at most a few hundred to thousand simulations, thus excluding standard Monte Carlo techniques.

In this context uncertainty quantification methods for shall be *non-intrusive* (i.e. based on runs of legacy codes) and *parsimonious* (i.e. using the smallest number of runs) while being able to address problems with $O(10)$, usually non Gaussian, input random variables.

Lecture 1: Sparse Polynomial Expansions for Uncertainty Propagation and Sensitivity Analysis

In the first lecture a general framework for UQ in engineering applications is introduced. Polynomial chaos expansions (PCE) and recent advances in sparse representations are presented to compute at low cost the PDF and moments of quantities of interest (QoI). Global sensitivity analysis, which aims at reducing the complexity of a computational model by determining which input parameters drive the uncertainty of the QoI are then introduced. It is shown how sparse PCEs allow for an efficient estimation of Sobol' sensitivity indices.

Lecture 2: Structural Reliability Methods for Engineering Risk Analysis

One of the important questions addressed by engineers is to evaluate the probability that a system of interest fails to fulfill some performance criterion due to uncertainties. Computing such a probability of failure is also known as *rare event simulation*, since the expected value is usually extremely small, say $10^{-6} - 10^{-3}$. In this lecture classical methods referred to as structural reliability methods are first introduced. Recent developments based on the use of Gaussian process modelling (a.k.a. Kriging) for building a surrogate of the performance function are then presented together with active learning algorithms.

Tutorial: UQLab

In this tutorial the (Matlab-based) uncertainty quantification software UQLab (www.uqlab.com) will be used to allow the students to get familiar with the different methods presented in the two lectures. Accordingly, the tutorial will be split into two parts, namely the use of PCE for sensitivity analysis, and the use of reliability methods.

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