Workshop on Partial Differential Equations with Random Coefficients

Weierstraß-Institut für Angewandte Analysis and Stochastik

Berlin, November 13 – 15, 2013

www.wias-berlin.de/workshops/pdeRand-2013

Organizers:

WIAS Research Groups:

Numerical Mathematics and Scientific Computing
Nonlinear Optimization and Inverse Problems
Interacting Random Systems

Young Scientist's Group:

Modeling of Damage Processes

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Welcome

Dear Workshop Participant,

Welcome to the Weierstrass Institute for Applied Analysis and Stochastics in Berlin. Given below is some general information regarding logistics and other arrangements for our workshop.

Entrance to the building will be provided showing your participant's badge. Please wear it. Sorry, but the receptionist is supposed not 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 TAPAS Y MÁS, Neue Grünstraße 17, 10179 Berlin (near underground station Spittelmarkt) on Thursday, November 14. at 7 p.m.

We wish you a pleasant stay at the Institute and in Berlin and look forward to an exciting workshop with interesting talks and lively discussions.

Kind regards,

Jürgen Fuhrmann, Dietmar Hömberg, Wolfgang König, Christiane Kraus
(Organizers)

Contents

1 Internet Access

Wifi

- If you want to use the **eduroam** access in the WIAS-wlan to access your home server, you must have configured the eduraom wireless connection of your computer according to the instructions of the IT of **your** institution. If you have done this, please choose the wlan eduroam to connect.
- If you want to use the WIAS-wlan to get access to the Internet, please ask *Anke Giese* for a voucher with an individual password and further instruction. Please note that after using this password at one computer it can afterwards only be used at **this** computer.

Computer Facilities

All workshop participants have the possibility to check emails in room no. 010, ground floor, opposite from the lecture room. Any workstation in this room may be used.

For log-in please use the following selections and input

`Please enter your user name:` **pderand** [OK]

`Please enter your password:` **pdeS*13$** [OK]

for log-out: either use the [Log out...]-selection on the root window or the [EXIT] button of the desktop.

Please be aware that this account is used by all workshop participants. So, don't leave any confidential data in its home directory. All left over data will be removed after the workshop.

2 Program

Wednesday, November 13	
08:30 – 09:00	Registration
09:00	Opening **Hermann G. Matthies (Braunschweig)** Parametric and stochastic problems – an overview of computational methods (Lecture I)
10:30 – 11:00	– Coffee Break –
11:00	**Robert Scheichl (Bath)** Numerical analysis of elliptic PDEs with random coefficients (Lecture I)
12:30 – 14:00	– Lunch Break –
14:00	**Fabio Nobile (Lausanne)** Stochastic collocation and multi level Monte Carlo methods for elliptic PDEs with random coefficients
14:45	**Alexey Chernov (Reading)** Convergence analysis for multilevel variance estimators in multilevel Monte Carlo methods and application for random obstacle problems
15:30 – 16:00	– Coffee Break –
16:00	**Oliver Ernst (Chemnitz)** UQ for groundwater flow
16:45	**Francesca Bonizzoni (Lausanne)** Low-rank techniques applied to moment equations for the stochastic Darcy problem with lognormal permeability
17:30	**Vincent Heuveline (Heidelberg)** Uncertainty quantification and high-performance computing: application to flow problems

Thursday, November 14	
09:00	**Hermann G. Matthies (Braunschweig)** Parametric quantities, their representations and factorizations, and inverse identifications methods (Lecture II)
10:30 – 11:00	– Coffee Break –
11:00	**Nicolas Dirr (Cardiff)** PDEs and variational problems with random coefficients (Lecture I)
12:30 – 14:00	– Lunch Break –
14:00	**Wolfgang Nowak (Stuttgart)** Freedom, subjectivity, robustness and in uncertainty quantification: What to do if the input statistics are uncertain?
14:45	**Anthony Nouy (Nantes)** Random fields representations for stochastic elliptic boundary value problems and high-dimensional statistical inverse problems
15:30 – 16:00	– Coffee Break –
16:00	**Werner Römisch (Berlin)** Convergence of solutions of approximate random equations
16:45	**Martin Eigel (Berlin)** Advances in adaptive stochastic Galerkin FEM
19:00	Dinner

Friday, November 15	
09:00	**Robert Scheichl (Bath)** Novel Monte Carlo methods and uncertainty quantification (Lecture II)
10:30 – 11:00	– Coffee Break –
11:00	**Nicolas Dirr (Cardiff)** PDEs and variational problems with random coefficients (Lecture II)
12:30	Closing

3 Abstracts of Minicourses

N. Dirr (Cardiff University, UK)

PDEs and variational problems with random coefficients

Introduction and Motivation

Modeling materials with heterogeneities on a small scale lead naturally to PDEs with random coefficients, as these heterogeneities are in general of a random nature. I will present several examples. Further I attempt to set a general framework for PDEs with random coefficients and introduce some of the questions one may ask about them.

Existence and non-existence

Drawing on nonlinear examples taken from interface evolution problems, I will present some existence and non-existence results where probabilistic arguments play a crucial role.

Uniqueness of minimizer

It is well known that adding (white) noise to an ODE can create to existence of a unique invariant measure while the ODE itself has several stable equilibria. In this lecture I will explain a similar situation in a calculus of variations problem with random coefficients: The deterministic equivalent has several minimizers, while a suitable random perturbation (time-independent) leads to a unique minimizer.

Random Homogenization

I give a brief overview of recent progress on the state of the art of homogenization of (mainly nonlinear) PDEs with random coefficients and important open problems.

H. G. Matthies (TU Braunschweig, Germany)

Lecture I: Parametric and stochastic problems – an overview of computational methods

Many methods originally developed for stochastic problems can be used in the more general context of parametric problems where we primarily think of problems described by ordinary or partial differential equations, and where the parameters are the coefficient (-fields) appearing in them.

In this overview of computational methods, emphasis is given to the vigorously developing field of functional or spectral approximations. Apart from the usual spatial and/or temporal discretization which is necessary to make the problem computational tractable, this view entails an additional discretization of the parametric or stochastic dependence. It will be shown how to discretize/represent the “input” to the problem, which possibilities exist to formulate the discrete problem, and which algorithms can be used. One important topic in this context is the question of whether a certain method is “intrusive”. It will be shown that most of the methods can be formulated in a “non-intrusive” way.

Lecture II: Parametric quantities, their representations and factorizations, and inverse identifications methods

Vector valued parametric quantities, and in particular vector valued random variables, are intimately associated with linear mappings. In this way factorizations like the singular value decomposition and the spectral decomposition of self-adjoint operators are directly connected to separated representations, examples of which are the Karhunen-Loève expansion and the smoothed white noise representation. These separated representations are key to new developments of numerical methods based on low-rank tensor approximations. They also form a good foundation for fast methods for inverse parameter identification procedures.

Parameter identification involves the observation of a function of the state of some system which depends on some unknown parameters. The mapping from parameter to observable is commonly not invertible, which causes the problem to be ill-posed. In a probabilistic setting the knowledge prior to the observation is encoded in a probability distribution which is updated according to Bayes’s rule through the observation, equivalent to a conditional (conditioned on the observation) expectation. To perform the update one has to solve the forward problem, propagating the parameter distribution to the forecast observable. The difference with the real observation leads to the update. It is common to change the underlying measure in the update, but here we update directly the random variables describing the parameters, thus changing the parameter distribution only implicitly. This is achieved by a functional approximation of the random variables involved. The solution of the forward problem can be addressed more efficiently through the use of tensor approximations. We show that the same is true for the inverse problem. Both the computation of the update map – a “filter” – and the update itself can be sped up considerably through the use of tensor approximation methods. The computations will be demonstrated on some examples from continuum mechanics, for linear as well as highly non-linear systems like elasto-plasticity.

R. Scheichl (University of Bath, UK)

Lecture I: Numerical analysis of elliptic PDEs with random coefficients

Stochastic modeling is one of the predominant ways to deal with uncertainty and lack of data, as well as to quantify the propagation of this uncertainty through the system to the real quantities of interest, such as the production rate of an oil well or the ultimate design load of an airplane wing made out of carbon fibre composites. At the heart of this process is in most cases the numerical solution of partial differential equations with random coefficients that represent the partially known and/or uncertain coefficients. In this first lecture I will motivate this problem with an example from subsurface flow: the safety assessment of a longterm repository for radioactive waste. The resulting mathematical problem is an elliptic PDE with random coefficients that are neither uniformly bounded away from zero nor from infinity and that lead to solutions that lack full regularity (globally). On the basis of this example we will discuss the typical questions of numerical analysis, such a s existence, uniqueness and regularity of solutions, as well as discretization via finite elements and their convergence in various norms. This includes the regularity with respect to the stochastic parameters which plays an important role for stochastic Galerkin and polynomial chaos type methods, as well as for quasi-Monte Carlo methods discussed in Lecture 2. The key difficulties in the analysis are the lack of spatial regularity, as well as the lack of uniform bounds on the diffusion coefficient. Another important point is that, by nature, random fields can only be evaluated approximately, leading either to quadrature or to some truncated spectral representations of the input data, and so we will also discuss variational crimes. We will finish the first lecture by discussing the extensions to finite volume schemes and to mixed finite elements, as well as to problems with discontinuous coefficients and random interfaces.

Lecture II: Novel Monte Carlo methods and uncertainty quantification

In this second lecture we will focus on algorithmic aspects and the complexity of algorithms. The ultimate goal of uncertainty quantification are typically some moments or the distribution of certain quantities of interest, such as the maximum load on an airplane wing or the "break-through timeöf a pollutant plume from the repository to the exterior of a safety region. Thus, the core numerical task is numerical integration over the stochastic parameter domain. We will analyses the ε-cost of typical algorithms to compute these statistics, i.e. the complexity to approximate them with an error of $O(\varepsilon)$ via quadrature. Many practical applications, such as the model problem developed in Lecture 1, necessarily lead to very high dimensional quadrature problems to capture the full (spatial/temporal) variability of the input coefficients. Many higher order methods, such as stochastic Galerkin or polynomial chaos approximations, suffer from the curse of dimensionality an d become prohibitively expensive in higher dimensions. Moreover, they rely on a smooth dependence of the solution (and often even an affine dependence of the differential operator) on the stochastic parameters. Again, these properties are not typically satisfied in many problems. The major workhorse in real applications remains the Monte Carlo method, i.e. simple sampling and averaging. It does not suffer from the curse of dimensionality and requires only minimal smoothness with respect to the stochastic parameters. However, its slow convergence of $O(N^{-1/2})$ with respect to the number of samples in combination with the typically high cost to compute individual samples in large scale engineering applications allow only very low accuracies in practice. I will describe two powerful remedies that can make Monte Carlo methods more efficient and more accurate: the multilevel Monte Carlo (MLMC) method and the quasi-Monte Carlo (QMC) method. These two variants are complementary and so they can even be combined. The MLMC method relies on a hierarchy of PDE discretizations and on their convergence, while the QMC method depends on sufficient smoothness with respect to the stochastic parameters. Based on the analysis from Lecture 1, we can give a full analysis of the complexity of both these variants for the subsurface flow model problem and show that they bring huge gains over the plain vanilla version. For rough input coefficients the MLMC method leads in fact to an asymptotically optimal method. I will finish the lecture by showing how the MLMC framework can also be extended to the inverse problem of quantifying the uncertainty given some data on the solution (in the form of some nonlinear functionals). In the stochastic setting this is referred to as Bayesian inference, and as in the forward problem, the main workhorse in applications is Monte Carlo in the form of the Markov chain Monte Carlo (MCMC) method of Metropolis and Hastings. I will present a multilevel MCMC algorithm and provide again a complete analysis for the subsurface model problem that confirms its superior complexity over the standard MCMC algorithm.

4 Abstracts of Research Talks

Low-rank techniques applied to moment equations for the stochastic Darcy problem with lognormal permeability

F. Bonizzoni (EPFL, Lausanne, Switzerland)
(joint work with: D. Kressner, R. Kumar, F. Nobile, C. Tobler)

The Darcy boundary value problem modeling the fluid flow in a bounded heterogeneous porous medium is considered, where the permeability is described as a log-normal random field. We perform a perturbation analysis, expanding the solution in Taylor series, and study the approximation properties of the Taylor polynomial, predicting the divergence of the Taylor series and the existence of an optimal degree of the Taylor polynomial such that adding new terms will deteriorate the accuracy. We approximate the expected value of the random solution with the expected value of its Taylor polynomial, and derive the recursive problem solved by the increasing order corrections of the expected value of the solution. This recursion involves the computation of high order correlations which, at the discrete level, turn to be high order tensors. To store and make computations we adopt a low-rank (tensor train) format.

Convergence analysis for multilevel variance estimators in multilevel Monte Carlo methods and application for random obstacle problems

A. Chernov (University of Reading, UK)

The Multilevel Monte Carlo Method (MLMC) is a recently established sampling approach for uncertainty propagation for problems with random parameters. In this talk we present new convergence theorems for the multilevel variance estimators. As a result, we prove that under certain assumptions on the parameters, the variance can be estimated at essentially the same cost as the mean, and consequently as the cost required for solution of one forward problem for a fixed deterministic set of parameters. We comment on fast and stable evaluation of the estimators suitable for parallel large scale computations.

The suggested approach is applied to a class of scalar random obstacle problems, a prototype of contact between deformable bodies. In particular, we are interested in rough random obstacles modeling contact between car tires and variable road surfaces. Numerical experiments support and complete the theoretical analysis.

Advances in adaptive stochastic Galerkin FEM

M. Eigel (WIAS Berlin, Germany)

Spectral Galerkin methods for PDE with stochastic data can exhibit high convergence rates according to the regularity of the stochastic solution. Due to the projection property and opposite to other methods based on polynomial chaos expansions, a posteriori error estimators and adaptive marking strategies similar to the deterministic case can be derived. We discuss some preliminary results concerning recent advances. The talk is based on joint projects with C.J. Gittelson, Ch. Merdon, C. Schwab and E. Zander.

UQ for groundwater flow

O. Ernst (TU Chemnitz, Germany)
(joint work with: B. Sprungk, H.-J. Starkloff, K. Andrew Cliffe)

We consider the problem of Darcy flow through a porous medium with lognormally distributed random conductivity field as a model of groundwater flow under uncertainty.

We review our recent work on uncertainty propagation using sparse grid stochastic collocation based on a statistical model of the input random field derived from conductivity observations for a specific radioactive waste storage application.

We will also present computational results for solving the stochastic inverse problem of estimating the input random field from measurements of hydraulic head. Basic considerations on different current stochastic inversion methods and their interpretation will also be discussed.

Uncertainty quantification and high-performance computing: application to flow problems

V. Heuveline (IWR Heidelberg, Germany)

Many fluid flow problems can be modeled by the incompressible Navier–Stokes equations. However, in practice knowledge for the description and definition of model relevant parameters, such as the kinematic viscosity or boundary and initial conditions, cannot be assumed to be available in a deterministic way. There are often uncertainties involved, which can be generated for example by inexact measurements or modeling assumptions. Taking such uncertainties into account by stochastic models results in a parameterization by a set of independent random variables. This leads to a blown up system size requiring the development of efficient numerical methods making use of high-performance computing.

We present a parallel stochastic Galerkin multilevel method using Polynomial Chaos for the solution of the steady incompressible Navier–Stokes equations with random parameters. The multilevel scheme only requires solutions of deterministic systems based on the mean operator, which makes the approach non-intrusive and feasible for use with existing program code for deterministic models. The parallelization is based on a domain decomposition for the spatial variable and a shared-memory approach for speeding up the computation of the stochastic Galerkin residuals. We evaluate the multilevel method by solving the "flow over a backward-facing step" problem in two spatial dimensions and the three-dimensional "Lid-driven cavity" with a focus on convergence properties and computational time.

Stochastic collocation and multi level Monte Carlo methods for elliptic PDEs with random coefficients

F. Nobile (EPFL, Lausanne, Switzerland)

In this talk we consider an elliptic PDEs with diffusion coefficient described as a random field. Focus will be devoted to the so called "log-normal" model.

We first review stochastic collocation (SC) approximation schemes that rely on an orthogonal expansion of the input random field in independent random variables. The solution of the PDE can then be approximated by a suitable multivariate polynomial function of the random variables, starting from point evaluations on a sparse grid of Gauss or Clenshaw-Curtis points. We present recent convergence results for optimized sparse grid constructions.

Although in principle convergence could be achieved even in infinite dimension (countable number of random variables), the convergence rate can be very slow, and worse that a plain Monte Carlo approximation, whenever the series expansion of the input diffusivity field converges very slowly, as it is the case, for instance for exponential type, or more generally only Lipschitz continuous, covariance functions. On the other hand, the convergence is in general very fast for very smooth fields.

In the second part of the talk, we propose an algorithm that combines a Multi Level Monte Carlo (MLMC) approach with stochastic collocation, to address the case of rough random fields. The stochastic collocation approximation is applied to a problem having a smoothed diffusion coefficient and used as a control variate in a Multi Level Monte Carlo simulation applied to original rough problem.

We present some preliminary analysis of the combined MLMC/SC method and present some numerical results showing the its effectiveness.

Random fields representations for stochastic elliptic boundary value problems and high-dimensional statistical inverse problems

A. Nouy (Ecole Centrale de Nantes, France)
(joint work with: C. Soize)

We present new results for the identification of random fields through statistical inverse problems involving a stochastic elliptic boundary value problem. A general class of non-Gaussian positive-definite matrix-valued random fields adapted to the statistical inverse problems is introduced and its properties are analyzed. Using a parametrization of the random fields in this class, a complete identification procedure is proposed. Since the class of random fields possibly contain random fields which are not uniformly bounded, a particular mathematical analysis of the parameterized stochastic elliptic boundary value problem is developed and dedicated approximation methods are introduced. The numerical solution of this parameterized stochastic problem provides an explicit approximation of the application that maps the parameterized general class of random fields to the corresponding set of random solutions. This approximation can be used during the identification procedure in order to avoid the solution of multiple forward stochastic problems. An approximation of the very high-dimensional solution map can be obtained using low-rank approximation methods. These methods exploit the tensor structure of the solution which results from the particular parametrization of the class of random fields.

Freedom, subjectivity, robustness and in uncertainty quantification: What to do if the input statistics are uncertain?

W. Nowak (Universität Stuttgart, Germany)
(joint work with: S. Oladyshkin, M. Sinsbeck)

In many real applications, uncertainty is vague, and exact distribution shapes for the random coefficients in PDEs are unknown. Uncertainty quantification methods should offer freedom to choose the shape of input distributions freely, without restrictions to a limited class of mathematically convenient parametric distribution families. This allows letting available data speak for themselves, and avoids subjective choices of specific assumed distribution shapes. Whether using this new freedom or not, the available data to represent or infer input distribution shapes are limited. Two issues arise here. First, limited data lead to estimation uncertainty concerning input distribution shapes. This uncertainty should be assessed and propagated, e.g., by Bayesian statistical approaches. Second, the estimation uncertainty for input distributions leads to a higher-level statistical error in uncertainty quantification. Using accurate numerical techniques for uncertainty propagation (e.g., high-order polynomial chaos expansions, PCE) may be useless if the higher-level error dominates over the error of numerical approximation. This effect can be shown to induce optimality ranges for expansion orders, and these optimality ranges depend on the level of knowledge concerning the input distributions. These topics are discussed and illustrated with examples from subsurface hydrology. One example considered is history matching for a well-known carbon dioxide pilot injection site in eastern Germany. The history matching is achieved by Bayesian filtering with a PCE-based surrogate model for the involved multiphase flow and transport equations.

Convergence of solutions of approximate random equations

W. Römisch (HU Berlin, Germany)

Approximations of random operator equations are considered, where the stochastic inputs and the deterministic operator equation are approximated simultaneously. Convergence in Distribution of approximate solutions to a weak solution of the original random equation is proved under reasonable assumptions. The result is applied to Galerkin approximations of a nonlinear elliptic PDE with random coefficients. Quantitative versions of the result and the case of linear elliptic PDEs are also considered.

5 List of Speakers

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Wednesday November 13	Thursday November 14	Friday November 15
08:30 – 09:00 Registration 09:00 – 10:30 **Opening** H. Matthies I	09:00 – 10:30 H. Matthies II	09:00 – 10:30 R. Scheichl II
10:30 Coffee Break	**10:30 Coffee Break**	**10:30 Coffee Break**
11:00 – 12:30 R. Scheichl I	11:00 – 12:30 N. Dirr I	11:00 – 12:30 N. Dirr II
12:30 – 14:00 Lunch Break	**12:30 – 14:00 Lunch Break**	**Closing**
14:00 – 14:45 F. Nobile 14:45 – 15:30 A. Chernov	14:00 – 14:45 W. Nowak 14:45 – 15:30 A. Nouy	
15:30 – 16:00 Coffee Break	**15:30 – 16:00 Coffee Break**	
16:00 – 16:45 O. Ernst 16:45 – 17:30 F. Bonizzoni 17:30 – 18:15 V. Heuveline	16:00 – 16:45 W. Römisch 16:45 – 17:30 M. Eigel	
	19:00 Dinner	