Workshop on Uncertainty Quantification for High-Dimensional Problems

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List of Talks

1 Adaptive methods for random PDEs: the interplay between spatial and stochastic sparsity (Markus Bachmayr)

Uncertainties in coefficient functions of partial differential equations can be modelled by taking these coefficients to be random fields. Expanding these random fields as function series with scalar random coefficients, one obtains formulations of random PDEs as deterministic problems depending on countably many parameters. In this form, these problems can be treated by stochastic Galerkin methods that combine sparse polynomial approximations in the parameters with suitable spatial discretizations such as finite elements. In this talk, we consider adaptive stochastic Galerkin methods for solving these problems that are designed to make use of multilevel structures with spatial localization in series representations of random fields. We will show how such structures, which correspond to a suitable choices of coordinates for representing random fields, lead to improved sparse approximability of solutions and operators jointly in space and parameters, and how this sparsity can be exploited by adaptive methods with near-optimal computational complexity.

2 Uncertainty aware surrogates in inverse problems (Aretha Teckentrup)

We are interested in the inverse problem of estimating unknown parameters in a mathematical model from observed data. We follow the Bayesian approach, in which the solution to the inverse problem is the distribution of the unknown parameters conditioned on the observed data, the so-called posterior distribution. We are particularly interested in the case where the mathematical model is non-linear and expensive to simulate, for example given by a partial differential equation. A major challenge in the application of sampling methods such as Markov chain Monte Carlo is then the large computational cost associated with simulating the model for a given parameter value. To overcome this issue, we consider using Gaussian process regression to approximate the likelihood of the data. This results in an approximate posterior distribution, to which sampling methods can be applied with feasible computational cost. In this talk, we will show how the uncertainty estimate provided by Gaussian process regression can be incorporated into the approximate Bayesian posterior distribution to avoid overconfident predictions, and present efficient Markov chain Monte Carlo methods in this context.

3 Iterative and multilevel methods for PDE-constrained optimization under uncertainty (Fabio Nobile)

In this talk we consider Optimal Control Problems (OCPs) constrained by random Partial Differential Equations (PDEs), where the expected value or other risk measures of a cost functional is minimized. We will first focus on iterative methods to solve the optimality system associated to the OCP once the underlying PDE and the probability space have been suitably discretized. Such optimality system is typically of very high dimension, characterized by N state PDEs, N adjoint PDEs, and a single optimality condition, where N is the total number of collocation points used to discretize the probability space. We present few preconditioning and multigrid

strategies to solve efficiently the optimality system and test them on several cases, including an OCP with box constraints and L^1 penalization on the control, and a risk-adverse OCP involving the smoothed CVaR risk measure. We then discuss how multilevel ideas and hierarchical approximations can be used in the the context of PDE-constrained OCPs under uncertainty adopting a combination technique approach, which requires solving the OCP for several low-fidelity discretizations of the PDE and quadrature formulae to compute the expected cost functional. All the computed solutions are then linearly combined to get a final approximation. We show some theoretical error estimates and present numerical results showing the efficacy of the approach.

4 Domain decomposition methods for large neural network in high dimensional nonlinear mechanics problems (Bojana Rosic)

Many engineering problems in nonlinear solid mechanics are characterized by anisotropic and heterogeneous material behavior, often governed by constitutive laws that are not fully understood. To address this lack of knowledge, the corresponding high-dimensional partial differential equations (PDEs) are parameterized by material constituents that are modelled by positive definite stochastic tensors on the corresponding manifolds. However, this approach significantly increases the dimensionality of the PDEs, making real-time solutions impractical for applications such as design optimization and control. Given that the primary objective in these problems is to predict uncertainty in the quantity of interest (QoI), we propose utilizing deep neural networks as efficient surrogate models. To further reduce the computational cost of constructing the neural network that maps input features to the QoI, we introduce the use of domain decomposition methods. This approach partitions the neural network vertically or horizontally into smaller sub-domains, allowing the global neural network model to be replaced by several local networks that are computationally less demanding. In this presentation, we will explore several methodologies for implementing this framework, accompanied by numerical examples relevant to mechanical engineering applications.

5 Dynamical adaptive state estimation of Hamiltonian systems (Federico Vismara)

This talk focuses on the inverse problem of reconstructing an unknown function u from a finite set of measurements, under the assumption that u is the output of a parameterized partial differential equation with unknown input parameters. Typically, the target function u belongs to an infinite-dimensional Hilbert space and the geometry of the solution set $\mathcal{M}$ is not known *a priori*. Moreover, if $\mathcal{M}$ evolves over time, suitably adapting the position of the sensors is crucial to ensuring an accurate reconstruction at all times. One way to reduce the complexity of the problem is to approximate $\mathcal{M}$ by a linear, finite dimensional subspace V *via* model order reduction techniques, and to search for an approximation $u^* \in V$ to the state u. In order to enhance the quality of the estimation, dynamical low-rank approximation techniques can be employed to adapt the reduced space V. This introduces additional challenges whenever the system is characterized by a Hamiltonian structure, which must be preserved in the reduction step. In this talk we will discuss how to address inverse problems for Hamiltonian systems by combining a structure-preserving, adaptive model order reduction strategy with dynamical placement of the sensors.

6 Scalable Sampling Method for problems with high-dimensional parameters (Evie Nielen)

In the last two decades, model order reduction has been established as an important tool for the solution of high-dimensional parametrized partial differential equations. However, even with the development and success of new methods that exploit machine learning tools, the problem of offline sampling remains. Most methods still rely on a random sampling of the parameter space, which especially in high-dimensional parameter spaces necessitates large amounts of training data. We explain a novel method, called the Polytope Division Method

(PDM) to determine where to sample, therefore reducing the number of sampling required. PDM splits the parameter space into polytopes and investigates the quality of the sample in the barycenter of each polytope.

7 Adaptive Tensor methods for Uncertainty Quantification and Parameter estimation in systems of parametric PDEs (Damiano Lombardi)

Parameter estimation and Uncertainty Quantification in time dependent systems of parametric PDEs are challenging as the computational burden to solve them is often prohibitive. In the present talk, we will discuss a low-rank adaptive solver to parsimoniously discretise a Bayesian filter. Given partial noisy observations of the system state, we will sequentially estimate the unknown parameters (and eventually the boundary conditions) of the system. The method is composed of two parts: an adaptive low-rank solver based on a multilinear GMRES and an interpolation step, which is based on the Galerkin projection on the basis computed by the low-rank solver. The interplay between these two steps contributes to alleviate the memory burden and provides a substantial acceleration of the Bayesian filter computation. This will enable the estimation of the a posteriori density of the parameters and the Uncertainty Quantification of the quantities of interest. Several examples will be presented, ranging from the estimation of the boundary conditions in a parabolic problem, to a more challenging 3D fluid-structure interaction problem.

8 The dimension weighted fast multipole method for scattered data approximation (Jacopo Quizi)

In this presentation we consider a shape uncertainty quantification problem where the objective is to reconstruct a solution-based linear output functional. This task leads to the challenge of approximating scattered data within a high-dimensional framework, where anisotropic behavior, that is, decreasing variation across different dimensions, comes to our aid. To efficiently solve the scattered data approximation problem, we introduce a novel dimension weighted black-box fast multipole method which embeds a sparse polynomial interpolation technique, tailored to account for the anisotropy in the data. A comprehensive analysis of our method is provided, which includes the derivation of rigorous error estimates that offer theoretical guarantees for the performance of the approach. The presentation is complemented by numerical studies.

9 The random timestep Euler method and its continuous dynamics (Jonas Latz)

ODE solvers with randomly sampled timestep sizes appear in the context of chaotic dynamical systems, differential equations with low regularity, and, implicitly, in stochastic optimisation. In this work, we propose and study the stochastic Euler dynamics - a continuous-time Markov process that is equivalent to a linear spline interpolation of a random timestep (forward) Euler method. We understand the stochastic Euler dynamics as a path-valued ansatz for the ODE solution that shall be approximated. We first obtain qualitative insights by studying deterministic Euler dynamics which we derive through a first order approximation to the infinitesimal generator of the stochastic Euler dynamics. Then we show convergence of the stochastic Euler dynamics to the ODE solution by studying the associated infinitesimal generators and by a novel local truncation error analysis. Next we prove stability by an immediate analysis of the random timestep Euler method and by deriving Foster-Lyapunov criteria for the stochastic Euler dynamics; the latter also yield bounds on the speed of convergence to stationarity. The paper ends with a discussion of second-order stochastic Euler dynamics and a series of numerical experiments that appear to verify our analytical results.

10 Statistical Learning Theory for Neural Operators (Jakob Zech)

In this talk, we discuss convergence rates for neural network-based operator surrogates, which approximate smooth maps between infinite-dimensional Hilbert spaces. Such surrogates have a wide range of applications and can be used in uncertainty quantification and parameter estimation problems in fields such as classical mechanics, fluid mechanics, electrodynamics, earth sciences etc. Here, the operator input represents the problem configuration and models initial conditions, material properties, forcing terms, and/or the domain of a partial differential equation (PDE) describing the underlying physics. The operator output is the corresponding PDE solution. Our analysis demonstrates that, under suitable smoothness assumptions, the empirical risk minimizer for specific neural network architectures can overcome the curse of dimensionality both in terms of required network parameters and the input-output pairs needed for training.

11 Maximum a posteriori testing in statistical inverse problems (Remo Kretschmann)

In many inverse problems, one is not primarily interested in the whole solution $u^\dagger$, but in specific features of it that can be described by a family of linear functionals of $u^\dagger$. In [1], we perform statistical inference for such features by means of hypothesis testing.

This problem has previously been treated by multiscale methods based upon unbiased estimates of those functionals [2]. Constructing hypothesis tests using unbiased estimators, however, has two severe drawbacks: Firstly, unbiased estimators only exist for sufficiently smooth linear functionals, and secondly, they suffer from a huge variance due to the ill-posedness of the problem, so that the corresponding tests have bad detection properties. We overcome both of these issues by considering the problem from a Bayesian point of view, assigning a prior distribution to $u^\dagger$, and using the resulting posterior distribution to define Bayesian maximum a posteriori (MAP) tests. The existence of a hypothesis test with maximal power among a class of tests with prescribed level has recently been shown for all linear functionals of interest under certain a priori assumptions on $u^\dagger$ [3]. We study Bayesian MAP tests bases upon Gaussian priors both analytically and numerically for linear inverse problems and compare them with unregularized as well as optimal regularized hypothesis tests.

References:
R. Kretschmann, F. Werner (2024). Maximum a posteriori testing in statistical inverse problems.

[2] K. Proksch, F. Werner, A. Munk (2018). Multiscale scanning in inverse problems. Ann. Statist., 46(6B), p.3569–3602, doi:10.1214/17-AOS1669.

[3] R. Kretschmann, D. Wachsmuth, F. Werner (2024). Optimal regularized hypothesis testing in statistical inverse problems. Inverse Problems 40, 015013.Gaussian

12 Sensitivity of uncertainty propagation, risk, and Bayesian inversion (Björn Sprungk)

For a probabilistic uncertainty quantification analysis of, e.g., a partial differential equation with uncertain coefficients we need to postulate a probability distribution for the unknown parameters. This distribution is often based on subjective knowledge or statistical estimation given experimental data. In this talk we investigate the sensitivity of the resulting distribution of the random solution with respect to perturbations in the input distribution for the unknown parameters. We prove a local Lipschitz continuity with respect to total variation as well as Wasserstein distance and extend our sensitivity analysis also to risk functionals of quantities of interest of the solution. Here, we provide a novel result for the sensitivity of coherent risk functionals with respect to the underlying probability distribution. Besides these sensitivity results for the propagation of uncertainty and risk, we also investigate the inverse problem, i. e., Bayesian inference for the unknown coefficients given

noisy observations of the solution. Although, well-posedness of Bayesian inverse problems is well-known (with respect to the observational data), we establish the local Lipschitz continuity of the posterior with respect to perturbations of the (again subjective) prior. We consider continuity in Wasserstein distance as well as with respect to several other common metrics for probability measures. However, our explicit bounds indicate a growing sensitivity of Bayesian inference for increasingly informative observational data.

13 Multilevel Monte Carlo Methods with Smoothing (Anastasia Istratuca)

We consider the computational efficiency of Monte Carlo (MC) and Multilevel Monte Carlo (MLMC) methods applied to elliptic partial differential equations with random coefficients. We make use of the circulant embedding procedure to sample from the aforementioned coefficient. Then, to further improve the computational complexity of the MLMC estimator, we devise and implement the smoothing technique integrated into the circulant embedding method. This allows to choose the coarsest mesh on the first level of MLMC independently of the correlation length of the covariance function of the random field, leading to considerable savings in computational cost.

14 Consensus-Based Rare Event Estimation (Elisabeth Ullmann)

We introduce a new algorithm for rare event estimation based on adaptive importance sampling. We consider a smoothed version of the optimal importance sampling density, which is approximated by an ensemble of interacting particles. The particle dynamics is governed by a McKean-Vlasov stochastic differential equation, which was introduced and analyzed in [Carrillo et al., Stud. Appl. Math. 148:1069-1140, 2022] for consensus-based sampling and optimization of posterior distributions arising in the context of Bayesian inverse problems. We develop automatic updates for the internal parameters of our algorithm. This includes a novel time step size controller for the exponential Euler method, which discretizes the particle dynamics. The behavior of all parameter updates depends on easy to interpret accuracy criteria specified by the user. We show in numerical experiments that our method is competitive to state-of-the-art adaptive importance sampling algorithms for rare event estimation, namely a sequential importance sampling method and the ensemble Kalman filter for rare event estimation. This is joint work with Konstantin Althaus and Iason Papaioannou (TUM).

15 Uncertainty quantification analysis of bifurcations of PDEs with random coefficients (Chiara Piazzola)

In this talk we address the forward uncertainty quantification analysis of random dynamical systems exhibiting bifurcations. The exposition discusses both, dynamical systems and uncertainty quantification, highlighting how analytical and numerical tools from both areas can be suitably combined. In particular, we will focus on the Allen–Cahn equation, a prototypical model problem in nonlinear dynamics that exhibits bifurcations corresponding to variations of a deterministic bifurcation parameter. Going beyond the state-of-the-art, we introduce a random coefficient in the linear reaction part of the equation, thereby accounting for random, spatially-heterogeneous effects. Importantly, we assume a spatially constant, deterministic mean value of the random coefficient. We show that this mean value is in fact a bifurcation parameter in the Allen–Cahn equation with random coefficients. Moreover, we show that the bifurcation points and bifurcation curves become random objects and propose to employ a generalized polynomial chaos expansion to approximate their statistical properties. We present numerical examples where we combine the popular software package Continuation Core and Toolboxes (COCO) for numerical continuation and the Sparse Grids Matlab Kit for the polynomial chaos expansion.
This is joint work with Christian Kuehn and Elisabeth Ullmann.

[1] C. Kuehn, C. Piazzola, E. Ullmann, Uncertainty quantification analysis of bifurcations of the Allen–Cahn equation with random coefficients, Physica D: Nonlinear Phenomena, 2024, https://doi.org/10.1016/j.physd.2024.134390

16 Uncertainty Quantification in Neurobiological Networks (Daniele Avitabile)

This talk presents a framework for forward uncertainty quantification problems in spatially-extended neurobiological networks. We will consider networks in which the cortex is represented as a continuum domain, and local neuronal activity evolves according to an integro-differential equation, collecting inputs nonlocally, from the whole cortex. These models are sometimes referred to as neural field equations. Large-scale brain simulations of such models are currently performed heuristically, and the numerical analysis of these problems is largely unexplored. In the first part of the talk I will summarise recent developments for the rigorous numerical analysis of projection schemes for deterministic neural fields, which sets the foundation for developing Finite-Element and Spectral schemes for large-scale problems. The second part of the talk will discuss the case of networks in the presence of uncertainties modelled with random data, in particular: random synaptic connections, external stimuli, neuronal firing rates, and initial conditions. Such problems give rise to random solutions, whose mean, variance, or other quantities of interest have to be estimated using numerical simulations. In addition to this forward Uncertainty Quantification problem, I will also present results of an inverse problem in which cortical data is used to infer parameter and states of the neural field model.
This talk presents joint work with Francesca Cavallini (VU Amsterdam), Svetlana Dubinkina (VU Amsterdam), Gabriel Lord (Radboud University), and Khadija Meddouni (Radboud University).

17 Exploiting locality in sparse polynomial approximations for parametric PDEs with an application to parameterized domains (Wouter van Harten)

We study how the choice of the representation of a parametric, spatially distributed boundary of an elliptic partial differential equation affects the efficiency of a polynomial surrogate for the parameter-to-solution map for the solution on a reference configuration. We focus on the possible improvements in convergence rates by exploiting locality in the basis expansion of the domain. Theoretical analysis demonstrates that basis expansions with specific locality properties, combined with certain mappings to the reference configuration, improve the convergence rate of polynomial surrogates compared to globally supported basis functions. Additionally, we conduct extensive numerical experiments to validate this finding, comparing the convergence behavior of mollifier-based and PDE-based mappings, and highlighting the differences between the two.

18 Projected data assimilation (Svetlana Dubinkina)

Ensemble data assimilation is unable to reduce the error estimate for high-dimensional systems when used with small ensemble size. A typical remedy is dimension reduction by localization. Though localization reduces the error substantially for both linear and nonlinear data-assimilation methods, the former ones considerably outperform the latter ones in a quasi-linear regime. We propose a further dimension reduction based on projection and show substantial error decrease of a nonlinear data-assimilation method in a challenging data-assimilation numerical setup with a small ensemble size and ample observations.

19 Bayesian shape inversion in acoustic scattering (Laura Scarabosio)

In the inverse problem of recovering the shape of a scatterer from measurements of its scattered field, we are interested in the role of the frequency on the stability of the reconstruction. We cast the problem in a Bayesian setting and use the Helmholtz equation to describe the physics. The role of the frequency is analyzed by studying the well-posedness of the Bayesian inverse problem in a frequency-explicit way. We discuss numerical methods to sample efficiently from the posterior, by combining sequential Monte Carlo sampling with a finite element

discretization on a reference configuration to avoid remeshing. Numerical results illustrate the effectiveness of our approach.

20 Uncertainty Quantification for High-Dimensional Systems - comparisons between physics-based and AI-driven approaches to real world applications in physics, chemistry, and life sciences (Peter Coveney)

I will discuss the quantification of uncertainty in predictive models arising in physics-based models and models based on machine-learning. Applications will include predictions of the impact of pandemics, the design of advanced materials, discovery of new drugs and the behaviour of turbulent fluids. The curse of dimensionality has hitherto circumscribed the systematic study of more complex natural and artificial systems but the advent of scalable approaches is now starting to change things. A paradigm case which is widely used within the scientific community across all fields from physics and chemistry to materials, life and medical sciences is classical molecular dynamics. I will describe how, using novel scalable UQ methods, we are now able to make global rankings of the sensitivity of quantities of interest to the many hundreds to thousands of parameters which occur in these models. In particular, we are able to rank the importance of all the interaction potential (force field) parameters which arise in molecular dynamics simulations. I will compare and contrast such approaches with the situation which pertains when attempts are made to replace these f orce fields with machine learned versions in the hope of making them more widely applicable.

21 Sparse polynomial chaos expansions for uncertainty quantification in applied sciences (Bruno Sudret)

Computational models (a.k.a. simulators) play a crucial role in modern engineering and applied sciences, allowing for the performance prediction and optimization of engineering systems. High fidelity simulations, such as finite element models, provide engineers with the ability to assess system performance in silico, thus significantly reducing the reliance on expensive physical experiments. However, the more complex the system, the more uncertain are its governing parameters, environmental and operating conditions. In this respect, uncertainty quantification (UQ) methods used to solve reliability, sensitivity or optimal design problems have gained interest in both academia and the industry in the last decade. Monte Carlo simulation is a well-known, brute-force method based on random number generation to solve such problems. It usually requires thousands to millions of simulations for accurate predictions though, which is not tractable with high-fidelity simulators. Surrogate modelling has become a powerful solution for overcoming this computational challenge. By creating an efficient approximation of a simulator's output, surrogate models leverage a strategically selected, limited set of simulation runs (the experimental design), and advanced learning algorithms. In this presentation, we focus on polynomial chaos expansions that allow us to construct an analytical approximation of the underlying input/output map of the simulator. Global sensitivity analysis (socalled Sobol' indices) can be also obtained analytically. Dedicated solvers leading to sparse expansions allow us to tackle high-dimensional problem (with $\mathcal{O}^{1-2}$ parameters) with the same amount of computer experiments. In the last part of the talk, we will introduce additional ingredients such as timeor frequency warping and nonlinear autoregressive models to handle problems with functional outputs, e.g. dynamical systems

22 Computational assessment of interacting errors in turbulent flow simulations (Bernard Geurts)

Turbulent flow is characterized by a wide spectrum of temporal and spatial scales, giving rise to complex dynamics. Turbulence of relevance to problems in Science and Engineering often cannot be resolved fully and coarsened approximate models for the larger scales are developed. An important reduced order modeling approach is

so-called large-eddy simulation (LES), which is motivated through the application of a spatial convolution filter to the incompressible Navier-Stokes equations.

Filtering of the nonlinear terms in the Navier-Stokes equations gives rise to a closure problem, which prompts the introduction of a sub-filter model. This model is designed such that the consequences of dynamic interactions among the various scales on the evolution of the larger scales are represented. In LES, several sub-filter models have been developed, each with their own consequences regarding the accuracy with which coarsened flows can be predicted. Moreover, the translation of an LES formulation into a computational model introduces additional approximations of a numerical nature. These two sources of error, i.e., the sub-filter modelling error and the discretisation error, together induce a total simulation error that needs to be understood and quantified.

In the presentation, the LES closure problem and the decomposition of the total simulation error into modelling and discretisation components will be described. We focus on the generic turbulence problem of homogeneous isotropic flow and compute the error landscape of eddy-viscosity models. From this, we infer optimal simulation conditions minimising the total simulation error. Computational optimisation of model parameters is illustrated, and the interchangeability of numerical dissipation and sub-filter model dissipation is analysed for discontinuous Galerkin discretization.