46th SpeedUp Workshop on "Uncertainty Quantification and HPC"

University of Bern, August 30 and September 1, 2016

The 46th SpeedUp Workshop focusses on **Uncertainty Quantification and HPC** in Bern. The program consists of a hands-on tutorial on Thursday, August 30 and the actual workshop with invited speakers and posters on Friday, September 1, 2017.

The invited talks illustrate various aspects of Uncertainty Quantification (UQ) which combines probability theory and statistics with physical processes in the real world. UQ problems include prediction, model validation, parameter estimation, data assimilation and inverse problems. It is a field of growing interest and this workshop tries to illustrate this with invited talks from different fields of application of UQ. These talks will be complemented by presentations on mathematical and methodological aspects of UQ.

Programme

Tutorial on Thursday, 31. August 2017

9:00 – 12:00	**Block A** **Maximilian Koschade** Technische Universität München **Hands-on Tutorial on Bayesian Multi-Level Monte Carlo** - Introduction to Multi-Level Monte Carlo for Uncertainty Quantification - Hands-on session: predicting the statistics of an expensive stochastic PDE solver using lower-fidelity, cheaper solvers Requirements: - General knowledge about the Python programming language - Laptop with a Unix/Linux operating system (for Windows user I recommend a Linux virtual machine) - Python3 with the following packages: to be announced (minimum requirement numpy and pymc3). I recommend using anaconda (as well as Jupyter notebook) and will provide an environment file from which automatically all dependencies can be installed
12:00 – 13:30	Lunch
13:30 – 16:30	**Block B:** **Marcel Schöngens** CSCS, Zürich/Lugano **Hands-on Tutorial on *ABCpy*** - ABCpy overview: philosophy, architecture, parallelism - Hands-on: Implementation of a simple example inference problem using ABCpy and Jupyter notebooks - Hands-on: Bring your own model calibration problem and solve it with ABCpy Requirements: - General knowledge about the Python programming language - Laptop with a Unix/Linux operating system (for Windows user I recommend a Linux virtual machine) - Python3 with the following packages pre-installed (pip install): ipython, jupyter notebook, abcpy

Workshop on Friday, 1. September 2017

9:00 - 9:30	*Registration and Coffee*
9:30 - 9:45	*Welcome*
9:45 - 10:30	**Gernot Plank** Technische Universität Graz **Personalized models of total heart function** Cardiovascular diseases are with a prevalence of 45% a major cause of death in the industrialized world. Despite steady therapeutic improvements, many cardiovascular diseases of high epidemiological relevance cannot be cured and are treated by mitigating symptoms. Image-based patient-specific models of cardiac function are a highly promising approach to comprehensively and quantitatively characterize cardiovascular function in a given patient. Such models are anticipated to play a pivotal role in future precision medicine as a method to stratify diseases, optimize therapeutic procedures, predict outcomes and thus better inform clinical decision making. Key challenges to be addressed are two-fold. Expensive computational models must be made efficient enough to be compatible with clinical time frames and generic models must be specialized based on clinical data which requires complex parameterization and data assimilation procedures.
10:30 – 11:00	**Speed-poster presentation**
11:00 – 11:30	*Break and Poster Session*
11:30 - 12:15	**Phaedon-Stelios Koutsourelakis** Technische Universität München **Physics-conversant machine learning: from molecular dynamics to stochastic PDEs** This talk is concerned with the development and adaptation of probabilistic machine learning strategies for the solution of various problems in physical modeling. It is consistent with the emergence of data-driven discovery, commonly referred to as the fourth paradigm in science, for extracting governing equations from data in cases where models (or closures) remain elusive.
12:15 – 13:45	*Lunch*
13:45 – 14:15	**General Assembly of the SpeedUp Society**
14:15 – 15:00	**Marcel Schöngens** CSCS, Zürich/Lugano **ABCpy: Approximate Bayesian Computation at Scale** ABCpy is a highly modular, scientific library for Approximate Bayesian Computation (ABC) written in Python. In enables domain scientists to easily apply ABC to their research without being ABC experts; using ABCpy they can easily run large parallel simulations without much knowledge about parallelization, even without much additional effort to parallelize their code. Further, ABCpy enables ABC experts to easily develop new inference schemes and evaluate them in a standardized environment, and to extend the library with new algorithms. These benefits come mainly from the modularity of ABCpy. We give an overview of the design of ABCpy, and we provide a performance evaluation concentrating on parallelization.
15:00 – 15:30	*Coffee Break*
15:00 – 15:45	**Andrea Barth** Universität Stuttgart ***Quantification of Uncertainty via Multilevel Monte Carlo Methods*** Multilevel Monte Carlo methods were introduced to decrease the computational complexity of the calculation of, for instance, the expectation of a random quantity. More precisely, in comparison to standard Monte Carlo methods, the computational complexity is (asymptotically) equal to the calculation of one sample of the problem on the finest discretization grid used. The price to pay for this increase in efficiency is that the problem must be solved not only on one (fine) grid, but on a hierarchy of discretizations. This implies, first, that the solution has to be represented on all grids and, second, that the variance of the detail (the difference of approximate solutions on two consecutive grids) converges with the refinement of the grid. In this talk, I will give an introduction to multilevel Monte Carlo methods in the case when the variance of the detail does not converge uniformly. The idea is illustrated by the calculation of the expectation for an elliptic problem with a random (multiscale) coefficient and then extended to approximations of discontinuous nature, e.g. Poisson noise.
15:45 – 16:30	**Oliver Fuhrer** MeteoSwiss, Zürich **Mostly sunny or partly cloudy? HPC and UQ challenges in weather forecasting** Weather forecasts are inherently uncertain and techniques to quantify this uncertainty within the strict time-to-solution requirements is a considerable high-performance computing challenge. This talk will outline current practice in high-performance computing and uncertainty quantification for weather forecasting and highlight some of the current outstanding challenges.
16:30 - 17:00	*Closing and Farewell Apéro*