NUMERICAL METHODS FOR UNCERTAINTY QUANTIFICATION

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EDITORIAL PREFACE

Computational Science and Engineering has emerged in the last years as an extremely powerful discipline able to simulate the behaviour and evolution of complex systems described by sophisticated mathematical models. All this is made possible by the rapid growth of computer power that we have witnessed in the last decades. With the increasing use of computational tools, comes also an increasing need of a systematic assessment of the reliability of computer simulations and quantification of all sources of uncertainties associated to them, including discretization errors, models inadequacy, incomplete knowledge of model parameters, etc.

Many engineering applications are well described by deterministic mathematical models derived from basic physical principles. However, uncertainty might arise in the input data of the mathematical model as forcing terms, boundary conditions, model coefficients, domain shape, etc., either because of an incomplete characterization and lack of measurements (epistemic uncertainty) or because of an intrinsic variability of the system (aleatory uncertainty). Computing statistics of the solution to the mathematical model, in presence of random input data, leads to high- or infinite-dimensional integration/approximation problems. This gives rise to new classes of formulations, which require new algorithms, new ideas, and new tools for their analysis, with numerous open questions to be addressed in future.

The workshop “Numerical Methods for Uncertainty Quantification” was held at the Hausdorff Center for Mathematics (HCM), University of Bonn, Germany, in May 2013 and aimed at showcasing different aspects related to Uncertainty Quantification in differential models and the most recent and important progresses in the field both at the theoretical and computational level. This special issue is composed of the articles based on new scientific results reported at this workshop as well as some subsequent developments. It consists of selected contributions with particular emphasis on the computational component. We thank the Editor-in-Chief, Professor Nicholas Zabaras, for his encouragement to prepare this special issue, and the Hausdorff Center for Mathematics, University of Bonn for the generous financial support, which made the workshop possible.

The special issue consists of five articles briefly described below.

- The work by P. Benner and J. Schneider is concerned with numerical simulation of a coplanar waveguide with dielectric overlay in presence of uncertainty. The electromagnetic model is represented by time-harmonic Maxwell’s equations with uncertain material parameters. This work explores performance of two computational methods—the stochastic collocation method and model-order reduction based on a proper orthogonal decomposition.

- E. Kostina and M. Nattermann consider in their work a class of parameter estimation problems in the form of a weighted least-squares minimization with constraints. The quality of estimated parameters is determined

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by confidence regions containing the true parameters with certain probability. The authors develop a second-order sensitivity analysis for quadratic approximation of the confidence regions and illustrate performance of the proposed approach in several numerical examples.

- The goal of the article by M. Mohammadi and A. Borzi is to investigate the accuracy of a spectral discretization of a deterministic optimal control problem subjected to the constraint given by the Fokker–Planck equation. This model problem originates from an Itô stochastic differential equation with the drift depending on the control function. The Fokker–Planck equation is posed in the unbounded domain justifying the discretization by Hermite functions. The analysis of the one-dimensional case shows spectral accuracy of the proposed method.

- The article by R. Pulch and E. J. W. ter Maten investigates the performance of two-model order reduction (MOR) strategies for linear dynamical systems with uncertain parameters. One is based on MOR for the stochastic Galerkin (SG) system where the polynomial chaos expansion is used to represent the state and output variables. Alternatively, a parametric MOR can be applied to the original full system and then SG method is used to solve the reduced-order model. Both methods are analysed and their performance illustrated in several numerical tests.

- The work by M. Sinsbeck and W. Nowak deals with optimization of quadrature rules that can be used within the stochastic collocation approach for forward uncertainty propagation. The set of quadrature points and weights is determined by a constraint optimization problem which can be solved by Gauss–Newton type algorithms. Limitations of the method are discussed and its performance is illustrated in numerical tests.