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Preface

Uncertainty quantification in simulation science

There has been recently an intense interest in *verification* and *validation* of large-scale simulations and in modeling uncertainty, as it is manifested by the many workshops that have been organized to address these issues. Verification is the process by which we ensure that the algorithms have been implemented correctly and that the numerical solution approaches the exact solution of the particular model – typically a partial differential equation (PDE). The exact solution is rarely known for real systems so "fabricated" solutions for simpler systems are typically employed in the verification process. Validation, on the other hand, is the process that determines how accurately is the mathematical model compared to the physical phenomenon simulated, so it involves comparison of simulation results with experimental data. Characterization of experimental inputs in detail is of great importance but of equal importance are the metrics used in the comparison.

Uncertainty quantification (UQ) is a complex subject but it can be roughly classified as numerical uncertainty and physical uncertainty. The former includes spatial and temporal discretization errors, errors in solvers (e.g., incomplete iterations, loss of orthogonality), geometric discretization (e.g., linear segments), artificial boundary conditions (e.g., infinite domains), etc. Physical uncertainty includes errors due to imprecise or unknown material properties (viscosity, permeability, modulus of elasticity, etc.), boundary and initial conditions, random geometric roughness, equations of state, constitutive laws, etc. Uncertainty can also be characterized as *epistemic*, i.e. reducible or as reducible. For example, given the current rapid advances in quantitative imaging technologies, the rock permeability of an oil reservoir could be measured much more accurately in the future – this is an example of epistemic uncertainty. However, even in this case, and certainly in many simulations of realistic configurations, uncertainty is irreducible beyond some level or scale, e.g., background turbulence – there are no absolutely quiet wind tunnels and the atmosphere or the ocean are inherently noisy environments.

Most of the research effort in scientific computing so far has been in developing efficient algorithms for different applications, assuming an ideal input with precisely defined computational domains. Numerical accuracy checks and error control via adaptive discretization have been employed in simulations for some time now, but mostly based on heuristics. With the field reaching now some degree of maturity, the interest has shifted to deriving more rigorous error estimators and posing the more general question of how to model uncertain inputs and how to formulate new algorithms in order for the simulation output to reflect accurately the propagation of uncertainty. To this end, the standard Monte Carlo approach can be employed but it is computationally expensive and it is only used as the last resort. The sensitivity method is an alternative more economical approach, based on moments of samples, but it is less robust and it depends strongly on the modeling assumptions. There are other more suitable methods for physical and biological applications. The most popular technique for modeling stochastic engineering systems is the perturbation method where all stochastic quantities are expanded around their mean value via a Taylor series. This approach, however, is limited to small perturbations and does not readily provide information on high-order statistics of the response. Another approach is based on expanding the inverse of the stochastic operator in a Neumann series, but this too is limited to small fluctuations. Bayesian statistical modeling has been used effectively in several different

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applications to deal with large uncertainties. At the heart of this framework is the celebrated Bayes theorem that provides a formal way of linking the prediction with the observed data. A non-statistical method, the polynomial chaos expansion and its variants, has received considerable attention in the last few years as it provides a high-order hierarchical representation of stochastic processes, similar to spectral expansions. An example of this method to constructing error bars for a three-dimensional heat transfer problem is shown in Fig. 1.

The most important goal of incorporating uncertainty modeling and its propagation in large-scale simulations is that it will lead to new *non-sterilized* simulations, where the input parameters and geometric domain have *realistic representations*. The simulation output will be denoted not by single points but by distributions that express the sensitivities of the system to the uncertainty in the inputs. This is a key element to reliability studies and will provide the first step towards establishing simulation-based certificates of fidelity of new designs. It will also be a valuable tool for experimentalists as it will quantify individual sensitivities to different parameters, thereby suggesting new experiments and instrumentation.

This special volume of JCP includes 14 papers that deal with various aspects of UQ in simulations. It addresses both numerical and physical accuracy, and presents different techniques and points of view as UQ is a new field and no consensus exists at the moment. The first few papers present primarily methods while the rest present applications including ocean modeling, porous media, chaotic dynamics, aeroelasticity, fluid mechanics and shock dynamics. The interested reader may also find useful material in two related publications with focus on computational fluid dynamics and on structural mechanics in [1,2], respectively. Similar material but with a broader range of applications can be found in [3].

The first paper by Oberkampf and Barone provides a verification and validation framework with comprehensive definitions and reviews of the main concepts. The specific topic addressed is validation metrics in comparing simulation results with experimental data. Clearly, the old way of graphical comparison is inadequate and the authors develop two specific validation metrics and demonstrate their effectiveness in three representative examples.

The second paper by Sen et al. addresses numerical uncertainty and develops a posteriori error estimators in conjunction with techniques in constructing global reduced basis. The latter is also very useful in studying physical uncertainty. A new natural norm is introduced and a fast computational procedure is presented along with two examples for a heat conduction and an acoustics problem.

The third paper by Ghanem and Doostan presents a new method for the characterization of stochastic processes given limited experimental data. The authors employ polynomial chaos expansions with corresponding coefficients which are themselves random variables obtained using a Bayesian inference scheme.

The fourth paper by Su and Lucor develops a new method for constructing covariance kernels for stochastic inputs, which are modeled as processes that vary in space. The authors derive a stochastic PDE that is

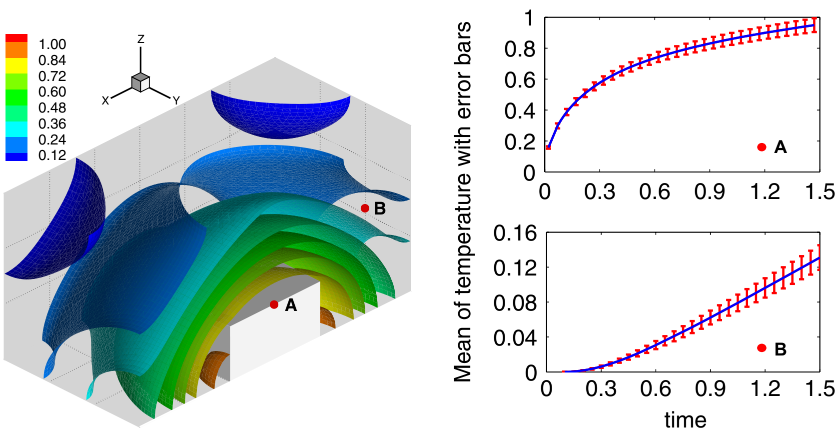

Fig. 1. Unsteady heat conduction with uncertain thermal diffusivity modeled by generalized polynomial chaos. The heat source is the cubic element shown in the 3D plot. (Left) Isosurfaces of standard deviation of temperature. (Right) Evolution of the mean temperature with error bars at two reference points. (Courtesy of Xiaoliang Wan, Brown University.)

forced by white noise and has the form of the Helmholtz equation. Different covariance kernels are derived for simple and complex geometries in multi-dimensions.

The fifth paper by Schwab and Todor also deals with modeling stochastic inputs using the Karhunen-Loeve representation. Here the focus is on resolving the covariance kernel fast, with almost linear work, by using a fast multipole accelerated Krylov eigensolver. The authors also derive accurate estimates of the convergence rate of the Karhunen–Loeve expansion in multi-dimensions.

The sixth paper by Dosteri et al. presents an efficient sampling strategy for the Markov Chain Monte Carlo (MCMC) method. The authors use inexpensive coarse-scale solutions to compute the gradients involved in the Langevin algorithms and prove that the modified MCMC converges to the correct posterior distribution given some mild technical conditions. Examples are presented for the permeability field.

The seventh paper by Christie et al. adapts a Bayesian framework to address uncertainty quantification in the context of oil reservoir simulations. The authors address the very real difficulties which arise, primarily the insufficiency of data, in this context and illustrate their ideas with specific examples.

The eighth paper by Park and Cushman models the dynamics of motile particles in random porous media with a hierarchy of stochastic differential equations. The multiscales are handled differently with the motile particle modeled as an operator stable Levy processes while at the macro scale the renormalized Fokker–Planck equations are employed.

The ninth paper by Winter et al. develops multivariate analysis of variance (ANOVA) methods to analyze the relation between heterogeneous and uncertain conductivities and the flow properties in an acquifer. ANOVA is performed on a large sample of Monte Carlo simulations.

The tenth paper is by Lermusiaux and addresses uncertainty modeling in ocean dynamics. The author reviews the many challenges involved in modeling interdisciplinary ocean processes and presents the error subspace statistical estimation (ESSE) method, which has been used with success in the Harvard Ocean Prediction System (HOPS) code. ESSE characterizes and predicts the largest uncertainties by evolving an error subspace of variable size that targets the more dominant errors.

The eleventh paper by Yu et al. addresses errors created within a simulation of a chaotic flow. The important issue here is that for chaotic flows, the simulation is underresolved, and since new structures are created on all length scales as the mesh is refined, convergence has to be interpreted in terms of averaged quantities. The central theme is to identify averages and statistical quantities which can be computed reliably.

The twelveth paper by Beran et al. considers the oscillations of an airfoil subject to variable (uncertain) torsional stiffness and to random initial conditions in the pitch angle. The authors consider the response of this stochastic dynamical system before and during the onset of the limit cycle oscillation, and in this context they evaluate several hybrid schemes that involve polynomial chaos and Haar wavelets as well as B-splines.

The thirteenth paper by Tartakovsky and Xiu considers geometric uncertainties in the form of random roughness pipe flow. The authors introduce a stochastic mapping that transforms the original flow problem in a domain with random boundary into another stochastic problem with deterministic boundary. They employ the generalized polynomial chaos to solve fast the resulting stochastic system and they compare their results against Monte Carlo simulations.

In the final paper, Lin et al. apply multi-element generalized polynomial chaos to supersonic flow past a wedge, a classical aerodynamics problem for which analytical solutions exist for the inviscid case. However, here the authors consider noisy inflow and random oscillations of the wedge around its apex and obtain new analytical solutions for small perturbations. They study convergence of this new method using the analytical solutions, and they extend their results to time-dependent noisy inflows.

We hope that this special issue of JCP will contribute to advancing stochastic modeling and motivate new work in UQ. We would like to thank all the authors and the referees for their contributions and Mr. Xiaoliang Wan (Brown University) who provided the results of Fig. 1. Finally, we are grateful to the chief editor of JCP, Gretar Tryggvason, for recognizing how timely and important is this subject.

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George Em Karniadakis
Division of Applied Mathematics, Center for Fluid Mechanics,
Brown University, 182 George Street, Box F,
Providence, RI 02912, United States
Tel.: +1 401 863 1217; fax: +1 401 863 3369
E-mail address: gk@cfm.brown.edu

James Glimm
Department of Applied Mathematics and Statistics,
P-138A Math Tower,
University at Stony Brook,
Stony Brook, NY 11794-3600
E-mail address: glimm@ams.sunysb.edu

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