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Computational Science and Engineering Workshop

Uncertainty Quantification in Computational Science

Abstract

Achieving predictive simulations of physical systems generally requires a concerted effort in verification and validation. In particular, assessment of model/code validity requires targeted comparisons against experimental measurements, with well characterized uncertainty/error bars in both experimental and computational results. This workshop will describe recent developments in uncertainty quantification (UQ) in computational science, focusing on the utilization of generalized polynomial chaos expansions (GPCE) for representation of random variables and processes, and the various means of forward propagation of uncertainty in the GPCE context in systems governed by partial and ordinary differential equations (e.g. applications in chemistry, thermofluids, materials, etc.). We will review Galerkin modeling in stochastic spaces, computational solution aspects, error estimation, and post-processing techniques, and cover both non-intrusive (sampling-based) and intrusive (direct) UQ methods. We will also discuss the utilization of Bayesian methods for estimation of uncertain parameters from data. Parameter estimation is a crucial element of any overall predictive simulation strategy, as the determination of well characterized uncertainties in model input parameters is a key step towards reliable UQ for model predictions. A number of current research topics on uncertainty quantification will finally be discussed, including interfacing multiscale and stochastic modeling, GPCE and Bayesian based stochastic optimization problems for systems governed by stochastic partial differential equations (SPDEs), UQ in oscillatory dynamical systems and flow fields, and others.

About Lecturers

Dr. Nicholas J. Zabaras is a Professor at the Sibley School of Mechanical and Aerospace Engineering at Cornell University. He received the Ph.D. degree in Theoretical and Applied Mechanics from Cornell University in 1987. His main research focus is on the development of mathematical, stochastic modeling and statistical techniques for materials by design. Recent research activities include multiscale design of materials processes and development of efficient ab initio based calculations for property and phase structure prediction. He has also contributed extensively on the development of GPCE, stochastic support, sparse grid collocation and Bayesian techniques for UQ in systems governed by SPDEs. His recent work in this area is on the development of data-driven reduced-order stochastic models. Dr. Zabaras is co-author of over ninety archival journal papers.

Dr. Habib N. Najm is a Distinguished Member of the Technical Staff at Sandia National Laboratories in Livermore, CA. He received the Ph.D. degree in Mechanical Engineering from the Massachusetts Institute of Technology in 1989. His work at the Sandia Combustion Research Facility covers a range of computational reacting flow research, with a focus on the development and utilization of advanced algorithms. He also works on the development of stochastic numerical methods for uncertainty quantification in thermofluid systems; on computational studies of stochastic dynamical systems and electrochemical microfluid systems; and on Bayesian statistics techniques for inverse problems and for analyte classification in micro/nano-channel biotechnology devices. Dr. Najm is co-author of over fifty archival journal articles and eleven US patents.

For more information, see http://www.cse.uiuc.edu/uq/
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