Stochastic Dimension Reduction Techniques for Efficient Uncertainty Quantification of Coupled Systems

Mathematical and Computational Tools for Predictive Simulation of Complex Coupled Systems Under Uncertainty

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Abstract

Predictive simulation of complex systems comprised of numerous interconnected components promises to help solve many problems of scientific and national interest such as the design, analysis, and licensing of of next-generation nuclear fission reactors. Achieving truly predictive simulation for these types of systems will require overcoming many fundamental mathematical and computational challenges including: (1) development of efficient coupling strategies for mixed-fidelity, multiple-scale system components through nonlinear solution processes; (2) accurately representing and efficiently propagating uncertainties through system components at multiple scales and levels of fidelity; (3) propagating uncertainty through the coupled system as a whole while adequately capturing critical couplings; and (4) solving stochastic inverse problems where probability distributions on stochastic inputs are determined to satisfy prescribed output statistics. To address these challenges, we propose a framework that integrates multiscale models, uncertainty quantification (UQ) and model validation. In particular, we investigate a computational framework to propagate uncertainty through system components based on a general stochastic expansion methodology. This approach includes both intrusive methods such as polynomial chaos and non-intrusive methods such as stochastic collocation, and allows head-to-head comparisons between methods discerning their relative advantages and disadvantages. Furthermore, we investigate an intrusive propagation approach similar to automatic differentiation, enabling automatic transformation to intrusive UQ-enabled simulation capabilities, as well as several linear solver and preconditioning approaches that improve the performance and scalability of the intrusive methods.

The computational cost of these expansion methods grows quickly with the stochastic dimension of the system, which in turn grows with the number of interconnected components. Therefore, we leverage this stochastic expansion framework to reduce the stochastic dimension of the uncertainty representation as it is passed from component to component in a coupled system. For "network" coupling where components are coupled through low dimensional interfaces, we discuss several dimension reduction approaches based on numerical generation of orthogonal polynomials and associated quadrature rules for random variables with arbitrary distributions. For higher-fidelity multi-physics coupling, we present an adaptation of Karhunen-Loève expansions to extract a lower dimensional representation of uncertainty as it crosses physics while mitigating the growth in stochastic dimension as uncertainties are stirred. This representation creates a de facto low dimensional interface between components for which the network techniques can then be applied. The effectiveness of these techniques is demonstrated on simple models of fission reactor cores consisting of coupled heat flow and neutron diffusion.