Propagating uncertainty from simulation parameters and sampling noise through coupled atomistic-to-continuum systems

Quantifying Prediction Fidelity in Multiscale Multiphysics Simulations

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Abstract

Multiscale multiphysics problems arise in a host of application areas of significant relevance to DOE, including electrical storage systems, water surety, chemical analysis and detection systems, and surface catalysis. Multiscale methods aim to provide detailed physical insight into these complex systems by incorporating coupled effects of relevant phenomena on all scales. However, many sources of uncertainty and modeling inaccuracies hamper the predictive fidelity of multiscale, multiphysics simulations. These include parametric and model uncertainties in the models on all scales, and errors associated with coupling, or information transfer, across scales/physics.

This project aims to identify and address key components of uncertainty quantification in spatially decomposed atomistic-to-continuum (AtC) multiscale simulations. These include inference of uncertain parameters or observables from experimental or simulation data; propagation of uncertainty through particle models; propagation of uncertainty through continuum models; propagation of information and uncertainty across model/scale interfaces; and numerical and computational analysis and control. This talk focuses on the multiscale simulation system and coupling of uncertain parameters across AtC interfaces, while presentations from other team members will detail other research aspects of this project.

A methodology is introduced to assess the predictive fidelity of multiscale simulations by incorporating uncertainty in the information transmitted between atomistic and continuum simulation components. The algorithm accounts for both noise due to finite MD sampling and contributions from parametric uncertainties while maintaining consistency between all uncertain variables. Surrogate models are introduced to limit the computational costs associated with MD sampling, and Bayesian inference is employed to build polynomial chaos expansions for variables exchanged across simulation model interfaces.

Two case studies are presented for laminar Couette flow, the first accounting for the effects of sampling noise (submitted to SIAM Multiscale Modeling and Simulation), and the second adding uncertain MD and continuum simulation parameters. The results demonstrate the ability of the approach to quantify uncertainty in coupled AtC simulations and illustrate how computational resource use can be controlled by targeting a desired level of uncertainty due to sampling noise. Finally, current work is presented outlining the application of this methodology to more complex mutiscale systems and uncertain long-range field effects.