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Quantifying Sampling Noise and Parametric Uncertainty in Atomistic-to-Continuum Simulations using Surrogate Models

Maher Salloum, Khachik Sargsyan, Reese Jones, Francesco Rizzi, Habib Najm, Bert Debusschere

Sandia National Labs, Livermore, CA

We present an approach for coupling atomistic and continuum solvers in multiscale simulations. In particular, we focus on systems with large separation in the relevant time and/or length scales of the atomistic and continuum phenomena, and account for uncertainty due to model parameters on the continuum and the atomistic level. Besides this parametric uncertainty, we also account for the uncertainty that is due to the use of a finite number of sample realizations for the extraction of macroscale quantities from atomistic simulations.

For computational efficiency, our approach constructs surrogate models or response surfaces for the coupling variables at the interface between the atomistic and continuum components, as a function of the uncertain parameters in the multiscale model. We use Bayesian inference to infer the atomistic surrogate model from short-time averaged data extracted from simulations at different values of the atomistic inputs. The resulting posterior uncertainty in this inferred surrogate model represents the uncertainty due to the finite amount of sampling from the atomistic simulations. The inferred response surfaces allow the efficient solution of a fixed-point problem that determines the coupling variables along with their associated uncertainty.

The approach is demonstrated on a canonical steady-state Couette flow case, with uncertainty in the atomistic force field model as well as in the continuum driving velocity. Sensitivity analysis shows that the main source of uncertainty is the atomistic force field parameter, with the sampling noise making only a minor contribution.

Overall, the surrogate model approach allows the quantitative assessment of the effects of sampling noise as well as other uncertainties on the predictive fidelity of atomistic to continuum simulations. If better confidence in the model predictions is desired, this approach also allows one to determine whether additional atomistic simulation data is needed to reduce the sampling noise, or if more information is needed to better quantify the input parameters.

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