Coupling Methods for Multiscale Simulations and Adaptive Modeling

Uncertainty Quantification in Atomistic-to-Continuum Methods for Complex Molecular Systems

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Abstract

In this talk, we will present our recent progress on the development of multiscale approaches for coupling concurrent models used to describe phenomena spanning different spatial scales. The main approach is based on the Arlequin framework in which a reference particle model, supposedly intractable, is replaced by a coupled model that blends solutions from small and large scale models [1,2]: more explicitly, a continuum (large scale) model is used far from the regions of interest and a particle (small scale) model is kept in the local critical regions. We will describe (1) a new coupling operator [3] that explicitly involves the size of the representative volume element (RVE) used to derive the continuum model from the particle model and show that it yields a well-posed formulation of the problem; (2) an alternative approach to a classical adaptive method [4] to automatically adapt the position of the coupling zone in order to reduce modeling errors with respect to quantities of interest; the new approach is based on optimal control [5]; (3) a novel approach for concurrently coupling non-local and local continuum models based on the peridynamics framework; and (4) an approach for the statistical calibration and validation of coarse-grained/continuum models and the stochastic coupling of models for uncertainty propagation. We will illustrate the theoretical results with recent numerical examples dealing with one- and two-dimensional problems.

References

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