Heterogeneous Multiscale Methods

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Simulating the most challenging multiscale problems requires interaction between different mathematical or physical models at different scales. Various computational techniques have been developed for improving coarse-scale models with with higher fidelity fine-scale or atomistic models. More traditional approaches have used a sequential strategy of precalculating finer-scale data and then using this information in a coarser model executed subsequently. Lately concurrent simulations, dynamically coupling models for different scales throughout the computation, have been developed. We will discuss computational aspects of these methods, for example. as they are applied to atomistic and continuum models in material science. The goal is to produce methods that have the accuracy of the fine-scale technique but with the computational complexity closer to a standard method for the coarse-scale.

One successful such technique is the quasicontinuum method by Tadmor and collaborators [1]. Local molecular dynamics simulations of a few representative atoms are inbedded in a finite element approximation in order to be able to model material responses on the continuum scale at zero temperature.

We will describe a general framework for these types of techniques called the heterogeneous multiscale method [2]. This framework can be used to develop coupled atomistic and continuum simulations at finite temperature. It can also be used to prove numerical convergence for simple applications. The basic principle is to derive, as detailed as possible, a computational algorithm for the macro-scale variables. The missing data in this model is then supplied on the fly by micro-scale simulations. The missing data could, for example, be a flux in a conservation law or an equation of state.

Two separate cases will be considered. In one there exists an effective equation that is valid in most of the domain. The macro-scale algorithm approximating this effective equation will then only need boundary data from the fine-scale simulation in the small domain where the effective equation was not adequate. In the other, there is no useful effective equation throughout the computational domain and fine-scale simulations will be performed in in a number of small sample sub-domains.

Some preliminary applications will be discussed.

References

[1] R. E. Miller and E. B. Tadmor. The Quasicontinuum method: Overview, applications and current directions. J. Comput-Aided Mater. 9:203-239, 2002. Available at: www.qcmethod.com/qcreview.pdf

[2] W. E and B. Engquist, The Heterogeneous Multiscale Method. Comm. Math. Sci., 1:87-133, 2003. Available at: intlpress.com/CMS/journal/v1i1/e.pdf See also the page www.math.princeton.edu/multiscale/ for many other applications.