Multiscale Methods and Its Applications to Nano-Mechanics and Materials

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ABSTRACT

Hierarchical and concurrent multiple scale modeling of heterogeneous systems and their governing equations are first derived followed by the development of hierarchical and concurrent multiscale simulation methods. These are fundamentally necessary to account for the multiple scale behavior observed in heterogeneous materials.

One of the most interesting questions in computational mechanics is: how do you make a connection between what is going on at the atomic scale and the material behavior at the macroscale? In many cases it is enough to write down an equation of motion for the large scales, letting all of the *averaged* atomic behavior be captured in parameters like the elastic moduli. However in some situations, like material fracture, the dynamics is dominated by atomic-scale behavior that cannot be captured with the standard material laws. In our proposed research, we are taking a multiple-scale method for these problems in which we seek to capture both the atomic-scale and macro-scale dynamics simultaneously. The proper coupling of these scales requires innovations based physics, statistical mechanics and novel numerical methods.

The above described heterogeneous materials systems all involve the concurrent coupling of dynamics at the atomic scale and the macroscale. The methods that we are developing to treat these problems must blend quantum and statistical physics with more conventional engineering concepts about continuum mechanics. We believe that it is only through this sort of multi-scale, multi-disciplinary approach that these problems in engineering today can be solved. As an added benefit, we aim to use our models and methods to assist in the design and analysis of nano-materials and nanostructures.

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