

Physical Mathematics Seminar

Multiscale Modeling of Materials

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Abstract

A number of complex physical phenomena require a description that spans several length scales and time scales, ranging from the atomistic to the macroscopic. Some representative examples include the fracture of ductile solids which can be strongly affected by chemical impurities, the electronic response of low-dimensionality systems with one (or more) dimensions at the nanoscale, and biological macromolecules which involve both mechanical and enzymatic behavior.

Methodologies that try to address such phenomena at all scales, concurrently or sequentially, are referred to as multiscale approaches. In this talk I will describe recent efforts to develop such methodologies and to apply them to representative systems of interest. While significant progress has been made, there are also many unresolved issues demanding the development of ever more sophisticated and accurate computational tools.



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