

Bridging Scale Methods for Nano Mechanics and Materials

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We demonstrate that the atomistic simulation tools are not sufficient for many of the interesting and fundamental problems that arise in computational materials design. These deficiencies lead to the thrust of multiple-scale methods. Hierarchical and concurrent multiple scale modeling of heterogeneous systems through the development of a set of coupled multiscale governing equations are then derived followed by the development of hierarchical and concurrent multiscale simulation methods for the solution of these equations. These are fundamentally necessary to account for the multiple scale behavior observed in heterogeneous materials. As an added benefit, we aim to use our models and methods to assist in the design and analysis of nano-materials and nanostructures, such as the Cybersteel, nano-composites, granular materials, fracture and shear bands, and bio-fluids.

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