Executive summary of my research on multiscale modeling and computation

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My research interest associated with multiscale modeling and computation is generally connected to mechanics and materials. Multiscale modeling and computation is in many ways to balance the desire for greater microscopic fidelity with the need for compact and efficient coarse-grained descriptions. This emerging research field has been identified as a major challenge and an absolute necessity for nanoscience and technology [1]. I have worked and published in this area in the past few years and the research efforts are summarized below.

1. Develop a novel quasicontinuum method using atomistic analysis to install constitutive realism and finite element to interpolate underlying material structures [2]. We have developed an adaptive way to pave the transition zone between atoms and finite elements for accurate force calculations. We have also extended application of the method to three dimensions with an efficient Delaunay mesh generator. Such extension allows us to study mechanical deformation processes at the sub-micron scale with atomistic fidelity [3].
2. Develop a concurrent multiscale modeling method using a continuum phase-field model [4]. The model is based on statistical mechanics and includes a phase-field that is proportional to the mass density and a displacement field governing by linear elastic theory. The added phase-field smoothes the sharp interface, enabling us to use equations of motion for the material grounded in basic physical principles rather than for the interface. The interface dynamics thus emerges naturally.
3. Develop a discrete element method to study dynamical behavior of colloidal particles at the nanoscale [5-6]. Simulations with combined actions of Brownian motion, effective DLVO inter-particle interactions in suspensions and imposed external fields are considered. This allows us to study the mechanisms behind assembly of nanoparticles in suspensions, and consequently its impacts on important technological applications (e.g., photonic bandgap crystals).
4. Develop a dissipate particle dynamics to study interfacial wettability between liquid, vapor, and solid phases [7]. The contact angle of a droplet on a solid platform is analyzed. This allows us to study mechanisms behind the profile of a micro-droplet, and consequently its impacts on important technological applications (e.g., transport phenomenon in NEMS devices).
5. Develop a software environment to cope with diversity and heterogeneity of multiscale modeling and computation [8]. We have constructed a software environment that provides flexible and expressive mechanisms for composing material descriptions and numerical kernels in order to experiment with different classes of models, algorithms, descriptions associated with multiscale modeling.

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