MAR16-2015-009429

Abstract for an Invited Paper
for the MAR16 Meeting of
the American Physical Society

Coarse-graining to the meso and continuum scales with molecular-dynamics-like models

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Many engineering-scale problems that industry or the national labs try to address with particle-based simulations occur at length and time scales well beyond the most optimistic hopes of traditional coarse-graining methods for molecular dynamics (MD), which typically start at the atomic scale and build upward. However classical MD can be viewed as an engine for simulating particles at literally any length or time scale, depending on the models used for individual particles and their interactions. To illustrate I'll highlight several coarse-grained (CG) materials models, some of which are likely familiar to molecular-scale modelers, but others probably not. These include models for water droplet freezing on surfaces, dissipative particle dynamics (DPD) models of explosives where particles have internal state, CG models of nano or colloidal particles in solution, models for aspherical particles, Peridynamics models for fracture, and models of granular materials at the scale of industrial processing. All of these can be implemented as MD-style models for either soft or hard materials; in fact they are all part of our LAMMPS MD package, added either by our group or contributed by collaborators. Unlike most all-atom MD simulations, CG simulations at these scales often involve highly non-uniform particle densities. So I'll also discuss a load-balancing method we've implemented for these kinds of models, which can improve parallel efficiencies. From the physics point-of-view, these models may be viewed as non-traditional or ad hoc. But because they are MD-style simulations, there's an opportunity for physicists to add statistical mechanics rigor to individual models. Or, in keeping with a theme of this session, to devise methods that more accurately bridge models from one scale to the next.