MAR17-2016-001365

Abstract for an Invited Paper
for the MAR17 Meeting of
the American Physical Society

Hierarchical Multiscale Simulation: Scale-Bridging for Shock Response of Energetic Materials

BRIAN BARNES, US Army Research Laboratory

As part of a multiscale modeling effort, we present progress on a challenge in continuum-scale modeling: the direct incorporation of complex molecular level processes in the constitutive evaluation. We use a concurrent scale-bridging approach, with a hierarchical multiscale framework running in parallel to couple a particle-based model (the lower scale) to the constitutive response in a finite-element multi-physics simulation (the upper scale). In this approach, many orders of magnitude in length scale separate the lower and upper scales, and the lower scale is able to be used in the constitutive model for all elements of the upper scale. Molecular level response includes the constitutive equation of state and non-equilibrium chemistry. Response dependent upon stochastic microstructure, such as porosity, and challenges for scale-bridging in time are also discussed. The lower scale simulations of hexahydro-1,3,5-trinitro-s-triazine (RDX) use a force-matched coarse-grain model and dissipative particle dynamics methods, and the upper scale simulates Taylor anvil and plate impact experiments. Results emphasize use of machine learning (via Gaussian process regression, or kriging) that accelerates time to solution, and its comparison to fully on-the-fly runs.

In collaboration with: Kenneth Leiter, Richard Becker, Jaroslaw Knap, John Brennan, US Army Research Laboratory.