Abstract Submitted
for the MAR16 Meeting of
The American Physical Society

Hierarchical Multiscale Framework for Materials Modeling: Advances in Scale-Bridging Applied to a Taylor Anvil Impact Test of RDX BRIAN BARNES, KENNETH LEITER, RICHARD BECKER, JAROSLAW KNAP, JOHN BRENNAN, 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. In this initial phase of the research we use a concurrent scale-bridging approach, with a hierarchical multiscale framework running in parallel to couple a particle-based model (the "lower scale") computing the equation of state (EOS) to the constitutive response in a finite-element multi-physics simulation (the "upper scale"). The lower scale simulations of 1,3,5-trinitroperhydro-1,3,5-triazine (RDX) use a force-matched coarse-grain model and dissipative particle dynamics methods, and the upper scale simulation is of a Taylor anvil impact experiment. Results emphasize use of adaptive sampling (via dynamic kriging) that accelerates time to solution, and its comparison to fully "on the fly" runs. Work towards inclusion of a fully reactive EOS is also discussed.

Brian Barnes
US Army Research Laboratory

Date submitted: 05 Nov 2015 Electronic form version 1.4