Abstract Submitted
for the SHOCK15 Meeting of
The American Physical Society

Coarse-Grain Modeling of Energetic Materials JOHN BRENNAN, U.S. Army Research Lab — Mechanical and thermal loading of energetic materials can incite responses over a wide range of spatial and temporal scales due to inherent nano- and microscale features. Many energy transfer processes within these materials are atomistically governed, yet the material response is manifested at the micro- and mesoscale. The existing state-of-the-art computational methods include continuum level approaches that rely on idealized field-based formulations that are empirically based. Our goal is to bridge the spatial and temporal modeling regimes while ensuring multiscale consistency. However, significant technical challenges exist, including that the multiscale methods linking the atomistic and microscales for molecular crystals are immature or nonexistent. To begin addressing these challenges, we have implemented a *bottom-up* approach for deriving microscale coarse-grain models directly from quantum mechanics-derived atomistic models. In this talk, a suite of computational tools is described for particle-based microscale simulations of the nonequilibrium response of energetic solids. Our approach builds upon recent advances both in generating coarse-grain models under high strains and in developing a variant of dissipative particle dynamics that includes chemical reactions.

John Brennan
U.S. Army Research Lab

Date submitted: 30 Jan 2015 Electronic form version 1.4