Abstract Submitted
for the SHOCK15 Meeting of
The American Physical Society

Nonholonomic Hamiltonian Method for Meso-macroscale Simulations of Reacting Shocks[1] ERIC FAHRENTHOLD, SANGYUP LEE, University of Texas at Austin — The seamless integration of macroscale, mesoscale, and molecular scale models of reacting shock physics has been hindered by dramatic differences in the model formulation techniques normally used at different scales. In recent research the authors have developed the first unified discrete Hamiltonian approach to multiscale simulation of reacting shock physics. Unlike previous work, the formulation employs reacting themomechanical Hamiltonian formulations at all scales, including the continuum. Unlike previous work, the formulation employs a nonholonomic modeling approach to systematically couple the models developed at all scales. Example applications of the method show meso-macroscale shock to detonation simulations in nitromethane and RDX.

[1]Research supported by the Defense Threat Reduction Agency

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Date submitted: 21 Jan 2015 Electronic form version 1.4