Abstract Submitted
for the SHOCK15 Meeting of
The American Physical Society

Nonholonomic Hamiltonian Method for Molecular Dynamics Simulations of Reacting Shocks[1] ERIC FAHRENTHOLD, JOSEPH BASS, University of Texas at Austin — Conventional molecular dynamics simulations of reacting shocks employ a holonomic Hamiltonian formulation: the breaking and forming of covalent bonds is described by potential functions. In general these potential functions: (a) are algebraically complex, (b) must satisfy strict smoothness requirements, and (c) contain many fitted parameters. In recent research the authors have developed a new noholonomic formulation of reacting molecular dynamics. In this formulation bond orders are determined by rate equations and the bonding-debonding process need not be described by differentiable functions. This simplifies the representation of complex chemistry and reduces the number of fitted model parameters. Example applications of the method show molecular level 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