Abstract Submitted
for the MAR05 Meeting of
The American Physical Society

A multi-scale method enabling long-duration molecular dynamics simulations of steady shock waves EVAN REED, LAURENCE FRIED, WILLIAM HENSHAW, Lawrence Livermore National Laboratory — A multi-scale simulation method is formulated and applied to the study of steadily propagating shock waves in materials. The method combines molecular dynamics and the Euler equations for compressible flow to provide up to 8 demonstrated orders of magnitude of computational savings over non-equilibrium molecular dynamics simulations of steady shock waves. The molecular dynamics system is constrained to obey the Rayleigh stress condition and the Hugoniot energy condition to sample the sequence of thermodynamic states of a steady shock. Utilizing a coarse- grained approach with analytical equations of state, we explicitly show that spatial profiles of shock waves yielded by the method are identical to those of fully hydrodynamic simulations of steady shock waves in chemically reactive systems.

Evan Reed
Lawrence Livermore National Laboratory

Date submitted: 06 Dec 2004 Electronic form version 1.4