

Abstract Submitted
for the SHOCK13 Meeting of
The American Physical Society

**Bridging the Scales from Molecular Dynamics to Navier-Stokes:
A Model of Nitromethane** CHRISTOPHER ROMICK, University of Notre
Dame, MARC CAWKWELL, TARIQ ASLAM, Los Alamos National Laboratory
— We present recent work on modeling liquid nitromethane from both a molecular
dynamics and continuum approach. Bulk properties of liquid nitromethane, includ-
ing isothermal compression, heat capacities, and viscosity have been computed from
a new quantum mechanical interatomic potential and classical force fields. These
bulk properties will be used to build a continuum-level model based in the com-
pressible Navier-Stokes equations. The two modeling paradigms will be compared
on a number of test problems.

Tariq Aslam
Los Alamos National Laboratory

Date submitted: 26 Feb 2013

Electronic form version 1.4