Abstract Submitted
for the SHOCK07 Meeting of
The American Physical Society

Hugoniot of complex fluids from molecular simulation: application to nitromethane EMERIC BOURASSEAU, CEA-DAM, ANAIS HERVOUET, NICOLAS DESBIENS, JEAN-BERNARD MAILLET, CEA-DAM, DPTA TEAM — The effect of molecular flexibility on the hugoniot shape is investigated using both MD and MC simulations. In the case of nitromethane, it is shown that molecular deformations with pressure play little role, and thus the rigid approximation may be used. A rigid model potential has then been fitted using a new technique, allowing fitting simultaneously several pressures on the hugoniot curve. This model is then used to simulate the behavior of nitromethane under shock conditions. Results are in good quantitative agreement with experimental data.

Jean-Bernard Maillet
CEA-DAM

Date submitted: 15 Feb 2007 Electronic form version 1.4