Abstract Submitted
for the DFD09 Meeting of
The American Physical Society

Accelerated Molecular Dynamics Simulation of Hypersonic Flow Features in Dilute Gases THOMAS SCHWARTZENTRUBER, PAOLO VALENTINI, University of Minnesota — Accurate simulation of high-altitude hypersonic flows requires advanced physical models capable of predicting the transfer of energy between translational, rotational, vibrational, and chemical modes of a gas in strong thermochemical non-equilibrium. A combined Event-Driven / Time-Driven (ED/TD) Molecular Dynamics (MD) algorithm is presented that greatly accelerates the MD simulation of dilute gases. The goal of this research is to utilize advances in computational chemistry to study thermochemical non-equilibrium processes in hypersonic flows. The ED/TD MD method identifies impending collisions (including multi-body collisions) and advances molecules directly to their next interaction, however, then integrates each interaction accurately using an arbitrary interatomic potential via conventional MD with small timesteps. First, the ED/TD MD algorithm and efficiency will be detailed. Next, ED/TD MD simulations of normal shock waves in dilute argon will be validated with experiment and direct simulation Monte Carlo simulations employing the variable-hard-sphere collision model. Profiling of the code reveals that the relative computational time required for the MD integration of collisions is extremely low and the potential for incorporating advanced classical and first-principles interatomic potentials within the ED/TD MD method will be discussed.

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Date submitted: 05 Aug 2009 Electronic form version 1.4