Abstract Submitted for the MAR08 Meeting of The American Physical Society

Large Scale Molecular Dynamics Simulations of Dense Plasmas. JEROME DALIGAULT, GUY DIMONTE, Los Alamos National Laboratory — Plasmas are generally created and probed by depositing energy into matter, driving it far from equilibrium. Knowledge over a wide range of physical conditions of the rate at which the electronic and ionic subsystems come into thermal equilibrium is important for explicit practical purposes. The microscopic mechanisms vary with the strength of the coupling among particles and the degree of degeneracy of the electrons. Though a variety of models for the electron-ion energy equilibration rate were proposed, these models apply to specific regimes, their range of validity and the transition from one regime to another remains unclear. Molecular dynamics (MD) simulations provide a powerful tool to investigate the validity of the various models. In order to study the temperature relaxation rates over a wide range of plasma coupling, from very weakly coupled to strongly coupled, multi-million particles simulations are necessary. To this end, we have developed a parallel MD code that employs the particle-particle particle-mesh algorithm and allow the simulation of very large, complex Coulomb systems and over long time scales. We have performed detailed, multi-million particle MD simulations to investigate and shed some new light on the electron-ion energy relaxation in hot, dense plasmas. In this talk, we will describe the MD code and discuss the original results obtained for the temperature relaxation rates.

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Date submitted: 11 Dec 2007

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