Molecular dynamics studies of electron-ion temperature equilibration in the coupled-mode regime

LORIN X. BENEDICT, MICHAEL P. SURH, CHRISTIAN R. SCULLARD, LIAM G. STANTON, ALFREDO A. CORREA, JOHN I. CASTOR, FRANK R. GRAZIANI, Lawrence Livermore National Laboratory, LEE A. COLLINS, JOEL D. KRESS, Los Alamos National Laboratory, CIMARRON COLLABORATION, T-1 COLLABORATION — We use classical molecular dynamics (MD) to study electron-ion temperature equilibration in two-component plasmas in regimes in which the presence of coupled collective modes substantively impacts the equilibration rate. Guided by previous kinetic theory work in which predictions were made of both the regimes and the sizes of this effect, we examine hydrogen plasmas at a density of $n = 10^{26} \text{ cm}^{-3}$, $T_i = 10^5 \text{ K}$, and $10^7 \text{ K} < T_e < 10^9 \text{ K}$. The non-equilibrium classical MD simulations are performed with inter-particle interactions modeled by quantum statistical potentials (QSPs). We compare our MD results to theoretical predictions using a Lenard-Belescu scheme, together with an accounting of time-varying potential energy (in the sense of a non-ideal, two-temperature equation of state), and discuss the extent to which our findings are expected to reflect those of true quantum hydrogen, as determined from quantum molecular dynamics simulations. This work is performed under the auspices of the U. S. Department of Energy by Lawrence Livermore National Laboratory under Contract DE-AC52-07NA27344 and by Los Alamos National Laboratory under Contract DE-AC52-06NA25396.

Lorin Benedict
Lawrence Livermore National Laboratory

Date submitted: 15 Jul 2016
Electronic form version 1.4