Abstract Submitted
for the DPP12 Meeting of
The American Physical Society

The Kinetic Theory Molecular Dynamics Method CHRISTOPHER FICHTL, MICHAEL MURILLO, Los Alamos National Laboratory, FRANK GRAZIANI, Lawrence Livermore National Laboratory, CIMARRON COLLABORATION — Plasmas under the thermonuclear burn conditions relevant to ICF and astrophysical plasmas typically consist of moderately degenerate, weakly coupled electrons and classical, moderately to strongly coupled ions. In order to better simulate such conditions, we have developed the Kinetic Theory Molecular Dynamics (KTMD) method to self-consistently describe the non-equilibrium electron dynamics using an appropriate kinetic equation while leaving the ion dynamics to MD. To simulate the plasma electrons, we have developed a many-fermion quantum PIC code capable of simulating conditions in which the phase space evolution of the plasma electrons in an initial Wigner distribution is accurately described by the quantum Vlasov (Wigner) equation. The plasma ions are followed using a recently developed MD code that utilizes a PPPM field solver specifically tuned to work in conjunction with the PIC field solver. The PIC and MD codes are coupled via the field equations such that the plasma electrons and ions act as source terms for the update equations of the opposite species. We present the basic ideas behind our approach, its associated implementation, and several physics benchmking results to demonstrate its feasibility.

Christopher Fichtl
Los Alamos National Laboratory

Date submitted: 13 Jul 2012 Electronic form version 1.4