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Kinetic Theory Molecular Dynamics FRANK GRAZIANI, JOSEPH BAUER, Lawrence Livermore National Laboratory, MICHAEL MURILLO, Los Alamos National Laboratory, CIMARRON COLLABORATION — Computational methods for simulating dense plasmas are limited by their inability to treat the dynamical quantum evolution of the electronic component. Based on the fact that electrons are typically weakly coupled but mildly quantum mechanical and the ions may be strongly coupled, we develop a method that combines a Wigner kinetic treatment of the electrons with classical molecular dynamics for the ions. We refer to this hybrid method as "kinetic theory molecular dynamics," or KTMD. Using the N-body Klimontovich equation for the electron-proton plasma, three variations of KTMD are obtained. The first approach yields a closed set of equations consisting of a mean field quantum kinetic equation for the electron one-particle distribution function coupled to a classical Liouville equation for the protons. The latter equation includes both proton-proton Coulombic interactions and an effective electron-proton interaction. This approach is then extended to incorporate strong electron-proton correlations through the Singwi-Tosi-Land-Sjolander (STLS) ansatz. A third variation of KTMD is proposed by again extending the mean field approach to include dynamically evolving particle correlations.

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