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Kinetic theory molecular dynamics for hot, dense plasmas M.S. MURILLO, C.A. FICHTL, LANL, F.R. GRAZIANI, J. GLOSLI, J. BAUER, LLNL — Plasma simulation methods can be categorized by the degree to which they treat the time dependence of the electrons. Common methods make a Born-Oppenheimer approximation in which the electronic structure is computed for fixed ions. However, many applications, such as energy exchange processes, require explicit treatment of the electron dynamics. As such, we have developed a new method that retains full quantal electron dynamics. We take advantage of the fact that electrons are typically weakly-to-moderately coupled, but degenerate, whereas the ions are typically strongly coupled and classical. This suggests a hybrid method in which we solve for the electrons using a quantum kinetic theory for moderately-coupled, degenerate electrons and a full molecular dynamics approach is used for the ions; we refer to our method as "Kinetic Theory Molecular Dynamics." This computational approach, and its associated numerical implementation, will be described using a mean-field Wigner kinetic approach coupled to ion dynamics. The non-linear interactions that involve the electrons, which populate a time-dependent Fermi-Dirac, are computed using a modified PIC approach. Extensions to this capability will be discussed as well as numerous examples, such as non-linear waves and instabilities, algorithms beyond mean-field, and its use as a tool for understanding dense fusion plasmas.

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