The Kinetic Theory Molecular Dynamics Method

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We are interested in simulating plasmas under conditions relevant to the National Ignition Facility and thermonuclear burn. Under these conditions, the plasma electrons are generally moderately degenerate, weakly coupled, and quantum mechanical, whereas the ions are known to be fully classical and are moderately to strongly coupled. As such, we have recently developed the Kinetic Theory Molecular Dynamics (KTMD) method, which attempts to take advantage of these properties under with the observations that: (1) molecular dynamics is very good at propagating classical particles and computes their correlations exactly and (2) kinetic theory is well developed for weakly coupled plasmas. Hence, the basic approach of KTMD is to describe the non-equilibrium electron dynamics fully with a kinetic equation while leaving the ion dynamics to MD.

The current version of KTMD self-consistently follows the time evolution of an initial Fermi-Dirac electron distribution via the Vlasov-Poisson system. Our method utilizes smoothed particle shapes within the KT framework to avoid the "Coulomb catastrophe" common to point electrons within the standard MD framework. An optimized Ewald method has been developed for the calculation of Coulombic forces.

We present several initial results obtained using the WPMD method and discuss future improvements to the code. These include a binary collision model within the Vlasov framework as well as the extension of the method to the quantum Vlasov (Wigner) equation.