Abstract Submitted
for the DPP19 Meeting of
The American Physical Society

Testing Thermal Conductivity Models with Equilibrium Molecular Dynamics Simulations of the One Component Plasma[1] BRETT SCHEINER, SCOTT BAALRUD, University of Iowa — Equilibrium molecular dynamics (EMD) simulations are used to calculate the thermal conductivity of the one component plasma (OCP) via the Green-Kubo formalism. These simulations address previous discrepancies between the OCP thermal conductivity calculated from EMD and non-equilibrium MD. Analysis of heat flux autocorrelation functions show that very long (6 x 10^5 ω_p^{-1}) time series are needed to reduce the noise level to allow accurate time integration. The new simulations provide the first accurate data in the range $0.1 < \Gamma < 2$, allowing the evaluation of thermal conductivity models in a regime where they are predictive. We test calculations of thermal conductivity using generalized Coulomb logarithms from the theories of Lee-More, Landau-Spitzer, Tanaka-Ichimaru, and Baalrud-Daligualt and find that only the latter two can reproduce the trend of the MD data for $0.1 < \Gamma < 10$. The results provide the first test of the Landau-Spitzer thermal conductivity using MD and indicate that transport theories must include the effect of particle correlations to properly model $\Gamma > 0.3$. None of the evaluated theories are found to accurately model the OCP for $\Gamma > 10$.

[1]This work was supported by the U.S. Department of Energy, Office of Fusion Energy Sciences, under Award No. DE-SC0016159.

Brett Scheiner
University of Iowa

Date submitted: 27 Jun 2019 Electronic form version 1.4