Abstract Submitted
for the DPP20 Meeting of
The American Physical Society

Simulating Warm Dense Plasmas with a Hybrid Molecular Dynamics - Quantum Hydrodynamics approach[1] DAVID MICHTA, University of Rochester, FRANK GRAZIANI, Lawrence Livermore National Lab, GREG HAMMETT, Princeton University, PETROS TZEFERACOS, University of Rochester
— Modeling the slowing-down of charged projectiles in warm dense matter (WDM) is of great interest to the design of ion-beam and intense laser experiments, e.g., in describing fast α-heating in ICF. This process is complicated by the electrons being moderately Coulomb-coupled and partially quantum-degenerate, while also dynamically screening the projectile. In this regime, ab initio Molecular Dynamics (MD) simulations are typically employed, and solve for the self-consistent quantum ground-state electron density for the ion configuration at each timestep using Density Functional Theory (DFT). Here, we describe a Quantum Hydrodynamics (QHD) approach, which treats the electrons as a fluid with forces derived from DFT, ensuring accurate equilibrium equation of state properties. We derive the QHD equations from first principles, connect them to the machinery of DFT, and describe the predicted linear response. We developed a parallelized simulation code that combines MD ions and QHD electrons, and simulated a stopping power experiment conducted at the Jupiter Laser Facility. By comparing with a quantum statistical potential MD code, we show favorable results for the QHD-MD approach. We discuss possible extensions into the FLASH code framework.

[1]This work was performed under the auspices of the U.S. DOE by LLNL under Contract DE-AC52-07NA27344

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Date submitted: 02 Jul 2020 Electronic form version 1.4