Abstract Submitted for the DPP20 Meeting of The American Physical Society

Multiscale Simulation of Plasma Flows Using Active Learning¹ JEFF HAACK, A. DIAW, K. BARROS, C. JUNGHANS, B. KEENAN, Y. W. LI. D. LIVESCU, N. LUBBERS, M. MCKERNS, R. S. PAVEL, D. ROSENBERGER, I. SAGERT, T. GERMANN, Los Alamos National Laboratory — Plasma flows encountered in high-energy density experiments display features that differ from those of equilibrium systems. Non-equilibrium approaches such as kinetic theory (KT) capture many, if not all, of these phenomena. However, KT requires closure information, which can be computed from microscale simulations and communicated to KT. We present a concurrent heterogeneous multiscale approach that couples molecular dynamics (MD) with KT in the limit of near-equilibrium flows. To reduce the cost of gathering information from MD, we use active learning to train neural nets on MD data obtained by randomly sampling a small subset of the parameter space. We apply this method to a plasma interfacial mixing problem relevant to warm dense matter, showing considerable computational gains when compared with the full kinetic-MD approach. We find that our approach enables the probing of Coulomb coupling physics across a broad range of temperatures and densities that are inaccessible with current theoretical models.

¹Research presented in this article was supported by the Laboratory Directed Research and Development program of Los Alamos National Laboratory under project number 20190005DR. Los Alamos National Laboratory is operated by Triad National Security, LLC, for the National Nuclear Security Administration of U.S. Department of Energy (Contract No. 89233218CNA000001)

> Jeff Haack Los Alamos National Laboratory

Date submitted: 29 Jun 2020

Electronic form version 1.4