

Abstract Submitted
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Fast and Accurate Transport Coefficients for Dense Plasma Applications¹ LUCAS J. STANEK, Michigan State University and Sandia National Laboratories, RAYMOND C. CLAY III, KRISTIAN BECKWITH, Sandia National Laboratories, LIAM STANTON, San Jose State University, MICHAEL S. MURILLO, Michigan State University — Mixing of high- Z ablator materials into thermonuclear fuel can spoil burn conditions. Understanding the impact, and controlling the mixing process requires a detailed knowledge of transport coefficients across wide plasma regimes; the ability to rapidly compute these properties in dense plasma mixtures remains a challenge. Existing microscopic models such as Kohn-Sham density functional theory molecular dynamics (KS-DFT-MD) and pair-potential molecular dynamics (PP-MD) can determine these transport properties; however, relatively speaking, the former requires many CPU hours while the latter typically does not. We use the Vienna Ab-initio Simulation Package (VASP) to generate KS-DFT-MD data for force matching with the Yukawa and EGS [1] pair-potentials; we see a preliminary speedup of 10^5 times. We plan to use the inexpensive PP-MD to aid in the design and interpretation of Z Machine experiments at Sandia National Laboratories. SNL is managed and operated by NTESS under DOE NNSA contract DE-NA0003525 SAND Number: SAND2019-7663 A

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