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Pair-potential approximations for many-body plasma physics.[1]
M. MARCIANTE, Los Alamos National Laboratory, L.G. STANTON, M.S. MURILLO, CMSE Department, MSU — Predicting properties of dense plasmas across wide parameters regimes requires the numerical solution of a many-body dynamical system whose properties depend on various underlying quantum processes. For this reason, high fidelity physics codes (e.g. DFT (orbital-free or Kohn-Sham), classical-map HNC and path integral MC) yield accurate information about the microphysical properties of dense matter. However, their computational cost restricts the simulations to a few tens to few hundreds of ions. To simulate larger systems while retaining an accurate kinetic description of ions, classical MD simulations make use of quantum-effective pair-potentials between the ions. Such potentials involve a small set of parameters, whose values are obtained from DFT calculations, and allow to simulate multi-species systems at much lower computational cost. In these models, bound electrons are usually approximated by an effective charge and free electrons are described as a continuous density. We have undertaken a detailed comparison of our DFT-informed pair-potentials, with results from higher-fidelity physics codes, including g(r), VACF Z(t), and interdiffusion coefficients, in order to determine the physical regimes in which the simpler accurate and very large-scale simulations are possible.

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Mathieu Marciante
Los Alamos National Laboratory

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