Abstract Submitted
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Particle-Particle-Particle-Mesh (PPPM) method generalized to arbitrary linear screening of Coulomb potential for large-scale simulation of strongly coupled plasmas G. DHARUMAN, Michigan State University, L. STANTON, J. GLOSLI, Lawrence Livermore National Lab, M. S. MURILLO, New Mexico Consortium — Molecular Dynamics (MD) simulation is a powerful method for studying large-scale correlated plasmas like warm dense matter, high-energy density plasmas and dusty plasmas. The bottleneck in MD is force calculation which naively scales as O(N^2) where N is number of particles which limits the length and time scales achievable. Depending on the nature of interaction between particles, forces can span short-intermediate-long range and efficient methods like Linked-Cell-list (LCL) [1] algorithm for short range forces scales as O(N) and PPPM [1] algorithm for long range forces scales as O(N log N). In some plasmas of interest, forces can be of intermediate range depending on screening, raising a question of which of the two algorithms needs to be used. We generalized PPPM to systems described by an arbitrary dielectric response function [2]. From this generalization we optimized to find a boundary in the space of simulation size and screening that demarcates PPPM from LCL in terms of computational efficiency. We examine the implications of different choices of screening function on the cost of computing dynamic structure factor that provides insight into plasma dynamics spanning small to large wavelengths and frequencies. [1] Computer simulation using particles, CRC press 1988 [2] Phys. Rev. E 91, 033104 (2015)

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