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Developing efficient MD method for strongly coupled plasmas[1]

JAWON JO, ERIC D. HELD, JEONG-YOUNG JI, Department of Physics, Utah State University, Logan, Utah, 84322 — Molecular dynamics (MD) is one of the most intuitive techniques to analyze a many-body system such as a plasma. It considers interactions of all particle pairs in the system and solves Newton's equations of motion to calculate statistical quantities such as temperature. A great strength of MD is adequately analyzing statistical phenomena of the system which we can't analytically. For example, we can observe the time evolution of temperatures of various species in a plasma and calculate their equilibration time. A weakness is a huge amount of computational effort, $O(N^2)$ for N particles, to compute all interactions. Several efficient methods are developed: The Ewald sum reduces the computational effort to $O(N^{3/2})$, the particle-particle/particle-mesh method of Eastwood and Hockney to $O(N \log N)$, and the fast multipole method of Greengard and Rokhlin to $O(N)$. In this work, we develop a hybrid method that computes particle-particle interactions for up to neighboring cells and adopts the fast multipole method for distant cells. The hybrid method significantly reduces the computational effort for a large number of particles, $N > 5 \times 10^4$. We present MD simulation results from studying temperature equilibration of two species for a strongly coupled plasma.

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