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Generalized Yukawa PPPM for molecular dynamics simulation of strongly coupled plasmas GAUTHAM DHARUMAN, Michigan State University, East Lansing, MI, USA, LIAM STANTON, JAMES GLOSLI, Lawrence Livermore National Laboratory, Livermore, CA, USA, JOHN VERBONCOEUR, ANDREW CHRISTLIEB, Michigan State University, East Lansing, MI, USA, MICHAEL MURILLO, Los Alamos National Laboratory, Los Alamos, NM, USA
— The Particle-Particle-Particle-Mesh (PPPM) method is an efficient way of treating the Ewald sum for long range interactions in a periodic system [1]. It makes use of the Fast-Fourier-Transform algorithm that scales as O(N logN). In this work we have applied the PPPM method to long range interactions in the weak screening limit of generalized Yukawa interaction to identify the range of screening over which PPPM is computationally more efficient than the minimum image method [2] which is usually usedfor the well-known Yukawa interactions [3]. Generalized Yukawa interaction is obtained by including arbitrary linear dielectric screening in the Yukawa model [4]. In the PPPM method the Fourier space part of the Ewald sum is treated by assigning charges to a mesh and computing the potential using an optimized Green's function that minimizes the discretization errors introduced in the forces [1]. [1] H.A. Stern and K.G. Calkins, J. Chem. Phys. 128, 214106 (2008). [2] M.P. Allen and D.J. Tildesley, Computer Simulation of Liquids (Clarendon, Oxford, 1987). [3] S. Hamaguchi, R.T. Farouki and D.H.E. Dubin, J. Chem. Phys. 105, 7641 (1996). [4] G. Dharuman, L. Stanton, J. Glosli, J. Verboncoeur, A. Christlieb and M.S. Murillo, ?J. Comp. Phys. (submitted).

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