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Hamiltonian hybrid particle-field molecular dynamics and its use with metainference.

Abstract

The computational cost of atomistic simulations limits the time and length scales that can be simulated, motivating the search for alternative methods. Hybrid particle-field methods are among these alternative methods that can be used to simulate systems that lie between the coarse-grain and mesoscale. Projecting the particles into densities distributed in a grid, one can eliminate the pair interactions and describe intermolecular interactions as a functional of the particle densities. In the Hamiltonian hybrid particle-field (HhPF) formulation [1], a particle-mesh formalism with filtered densities is used, achieving the conservation of energy and momentum, and an alias-free force computation. In this talk, I will introduce the HhPF method and its implementation in the Hylleraas MD [2]. Furthermore, I will show how the soft interactions produced by the method can be exploited together with the Metainference Bayesian method to bias simulations and obtain agreement with small angle scattering experiments [3].

References

[1] Bore and Cascella. Journal of Chemical Physics, 153, 094106(2020)

[2] Ledum et al. Journal of Chemical Theory and Computation, 19, 2939 (2023)

[3] Cezar and Cascella. Journal of Chemical Information and Modeling, 63, 4979 (2023)