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Efficient Hybrid Particle-Field Model Schemes for Large Scale Parallel MD Simulations

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In recent years, the success of and insight gained by classical molecular modeling, in understanding the fundamentals of complex molecular phenomena, have triggered a strong desire to go beyond the limitations of the information that can be extracted from classical Molecular Dynamics MD, especially the limitations that cannot be resolved by advances in computational efficiency. To this aim effective molecular representations have been developed and used for diverse molecular systems in a variety of coarse-grained (CG) and multi-scale (MS) techniques. (For a recent review and perspective see [1]) In the last decade, hybrid particle-continuum approaches such as Single-Chain in Mean-Field (SCMF) [2] and Hybrid Particle Field MD (hPF-MD),[3,4] which link discrete (particle-based) and continuum (field-based) descriptions in a single simulation volume, have been increasingly applied and validated for different systems. In hPF-MD, the nonbonded forces acting on a particle are expressed as function of the derivatives of local density gradients. This reformulation enables much more efficient simulations, especially for large parallel runs, than standard MD as the evaluation of nonbonded pair forces is replaced by building particle-to-mesh density fields and computing the density field potentials. Both steps are of first order in the number of particles. The hPF-MD model has been demonstrated to be effective to investigate homopolymers and block copolymers at both CG[5] and atomistic resolutions [6] also in the presence of solid nanoparticles [7-9] and for liquid-vapor interfaces [10]. The hPF-MD model was also validated in describing the conformational and dynamical properties of biological systems such as lipid bilayers[11-13], biosurfactants [14] and proteins [15]. More recently, after the integration of electrostatics into the hybrid particle-field scheme [16], the hPF-MD method was further successfully applied to charged phospholipids [17]. During the talk, after an introduction to the basics of hPF-MD methodology, I will give an overview of the main results with a special focus on electrostatic interactions their implementation and its applications from simple idealized to complex molecular models [18].

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