New simulation approaches for charged colloidal systems

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In order to simulate systems of charged colloidal spheres, we take the counterions explicitly into account, and model the hydrodynamic interaction by a dissipative coupling of extended spheres composed of point particles to a lattice Boltzmann simulation representing the solvent fluid. We present arguments why we believe this approach is useful, and present some numerical results for charged systems.

In a similar spirit, we attempt to replace the long-range electrostatic interaction between charges by a local coupling to a propagating electric field, such that the interaction is retarded. Constructing a Molecular Dynamics scheme along the lines of the Car-Parrinello approach, we find that this idea naturally leads to the solution of Maxwell's equations in a nonrelativistic version, where the speed of light is a tunable parameter, and the simulation lattice provides the role of an ether. Self-interaction problems resulting from the charge interpolation onto the lattice are solved by a suitable electrostatic subtraction, plus a suitable modification of the equations of motion. It is shown that this method yields correct thermal averages. Some numerical results are presented.