

# Simulating electrohydrodynamics in charged colloidal dispersions: A smoothed profile method

K. Kim, Y. Nakayama, and R. Yamamoto

PRESTO, JST and Department of Chemical Engineering, Kyoto University, Kyoto 615-8510, Japan

A new computational method is presented to study dynamical properties of charged colloidal dispersions. From a computational point of view, fully microscopic simulations are prohibitively inefficient because of the huge asymmetries both in size and time scales between colloidal particles (large and slow) and ions (small and fast). We accordingly propose hybrid type simulations consisting of particles which moves freely in space and a coarse-grained continuum density of ions which is discretized into grid points. However, this approach is a demanding task because of the mathematical singularities at the colloid-solvent boundaries and the numerical inefficiency associated with the moving boundary conditions. To overcome the difficulties, we introduce the smoothed profile for colloid-solvent boundaries [1, 2, 3, 4]. This smoothed profile method enables us to use the conventional Cartesian grid for many particle systems, which benefits the performance of numerical computations.

We especially focus on developing a simulation scheme applicable to realistic dynamics in many practical problems including electrophoresis for example. In such systems, the coupling between hydrodynamics and electrostatic interactions are crucial. Recently, in order to resolve the hydrodynamic interaction in colloidal dispersions, several semoscopic simulations such as Lattice Boltzmann method, Dissipative Particle Dynamics or Stochastic Rotation Dynamics have been proposed. On the other hand, in our method the background velocity field is given by solving Navier–Stokes equation directly [3] and therefore hydrodynamic effects can be fully taken into account. The time evolution of ion density is determined by coupling equations of hydrodynamics and thermal diffusion, and positions of colloidal particles are updated by solving equations of motion.

We performed simple demonstrations of electrophoresis, which are shown in Figure 1. We applying an external electric field to the system, a charged colloid moves with the constant velocity, which is determined by the balance between the electrostatic and viscous forces acting on the colloid. In Figure 1, it can be seen that for small electric field electric double layer is almost isotropic, while for large electric field electric double layer deforms and becomes anisotropic since ions in double layer cannot follow the colloid. Such a deformation of the double layer is known as the phenomenon of relaxation effect.

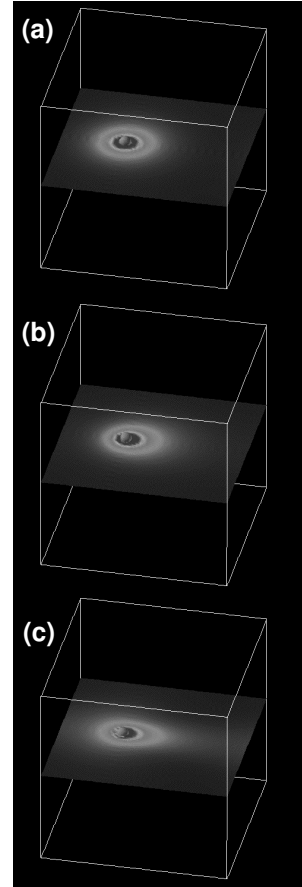


Figure 1: Snapshots of electrophoresis situation of a charged colloids with an applied electric field of (a)  $E = 0.01$ , (b)  $E = 0.1$ , and (c)  $E = 0.5$ . The charge density around the colloid is shown with a gray-scale map.

## References

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