Simulations of electrophoresis in charged colloidal dispersions: Smoothed profile method

JST PRESTO and Dept. of Chemical Engineering, Kyoto Univ.
Kang Kim[1], Yasuya Nakayama, and Ryoichi Yamamoto

コロイド分散系に対する効率的なシミュレーション方法であるSmoothed Profile法を用いて、荷電コロイド分散系の電気泳動シミュレーションを開発する。Smoothed Profile法はNavier–Stokes方程式を直接数値計算することで流体力学相互作用を解決しているシミュレーション手法であり、特に静電相互作用と流体力学相互作用の競合が重要である荷電コロイドの電気泳動現象に対して有用である。本発表では荷電コロイド分散系に対するSmoothed Profile法を概観し、3次元系での電気泳動シミュレーションについていくつかのデモンストレーションを紹介する。

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 disretized 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. In our method, the background velocity field is given by solving Navier–Stokes equation [3] and the time evolution of ion density is determined by coupling equations of hydrodynamics and thermal diffusion. In addition, positions of colloidal particles are updated by solving equations of motion.

We performed simple demonstrations of electrophoresis situation, which is shown in Fig. 1. We applying an external electric field to the system, a charged colloid starts to move with a constant velocity. In Fig. 1, it can be seen that for small electric field electric double layer is almost

---

[1] E-mail: kin@cheme.kyoto-u.ac.jp

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.

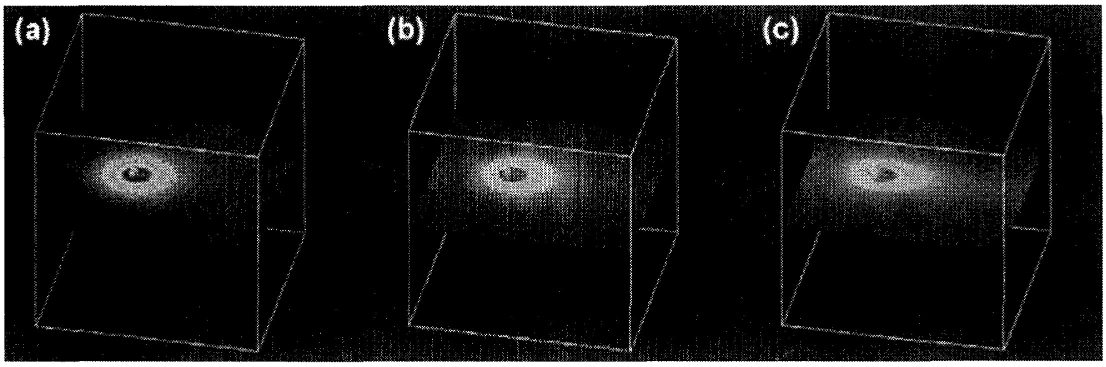

Figure 1: Snapshots of electrophoresis situation of a charged colloids with an applied electric field of (a)$E = 0.01$, (b)$E = 0.1$, and (c)$E = 0.5$. The charge density around the colloid is shown with a gray-scale map.

References

[1] R. Yamamoto, Phys. Rev. Lett. **87** (2001), 075502.

[2] R. Yamamoto, Y. Nakayama, and K. Kim, J. Phys.: Condens. Matter **16** (2004), S1945.

[3] Y. Nakayama and R. Yamamoto, Phys. Rev. E **124** (2005), 036707.

[4] K. Kim and R. Yamamoto, Macromol. Theory Simul. **14** (2005), 278.