Hydrodynamic effects in colloidal dispersions studied by a new efficient direct simulation

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Understanding properties of flowing colloidal suspensions is quite important both in scientific and engineering viewpoints. It includes the rheological problems, phoretic tranport of charged colloids, kinetics of aggregating colloids, and so on. However, the flowing colloidal systems is difficult to quantify experimentally or to predict theoretically.

Inter-particle interactions in suspensions consists of direct interactions and interactions mediated by solvent. The direct inter-particle interactions affects the flow of solvent which at the same time counteract on colloids. Moreover, internal microstructures of solvent induce effective inter-particle interactions and change the flow of solvent dramatically. The interaction mediated by solvent is essentially dynamical phenomenon and a key factor in understanding flowing collodal systems. However, fundamental understanding of dynamical behavior of colloids is limited to simple systems. Therefore, numerical simulations can be useful tools to extend the understanding such a complex problems in colloidal dispersions.

We developed a numerical scheme to simulate colloidal dispersions in complex fluids, named "Smoothed Profile method"(SP method). In Smoothed Profile method, material transport and flow of solvent is solved by hydrodynamic equations and motions of colloids are solved in the manner of classical molecular dynamics simulation. In conventional methods, moving solid-fluid boundary conditions and evaluation of force acting on colloids demands complex algorithms and/or huge computational resouces. The algorithm of SP method is designed to circumvent such complexity and inefficiency of conventional approach. In SP method, the solid-fluid interface is expressed as diffuse interface. SP method is a way to deal with moving boundary conditions and to evaluate forces on colloids both efficiently and accurately. By using SP method, many-colloid systems can be simulated without neglecting many-body interaction mediated by solvent, such as hydrodynamic interactions.

Figure 1 shows binary mixture of big and small particles.The concentration of small particles is indicated gray-scale, the darker the gray corresponds to a higher the concentration. The interaction between big and small particles is short-range repulsion. Small particles are driven from left to right. Each big colloid feel the osmotic force due to concentration gradient around its surface. Note that hydrodynamic interaction is fully considered and the concentration distribution is determined by the balance between the diffusion and the hydrodynamic friction. In this non-equilibrium situation, the effective interaction is directly computed in SP methods.

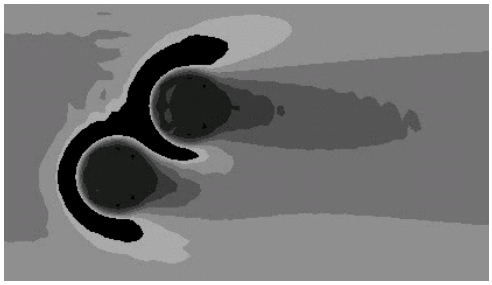

Figure 1: Binary mixture of big and small particles. Two big colloids are immersed in a solution of small particles.

Application of SP method to many-colloid systems and extension to complex solvent such as electrolyte solutions, liquid-crystal solvent are straightforward and now underway. We will discuss the hydrodynamic effects in colloidal suspensions.

References

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