

Technical Summary of PhD Thesis: Fast Simulation Methods for Soft Matter Hydrodynamics

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Soft materials and complex fluids comprised of colloidal particles or dissolved polymers are common to many industrial applications. The dynamics of these materials are determined by the structure and interaction of the constituent elements. Many applications of interest (e.g. gelation, crystallization, structure formation) involve either kinetic arrest or dynamic self-assembly; processes with kinetic pathways dictated by the Brownian motion characteristic of micron-scale elements and the fluid-mediated coupling of particle motion, called hydrodynamic interactions. In these applications, the coordinated motion of many particles across large length scales gives rise to emergent microstructure and macroscopic transport properties. Therefore, large simulations with many particles, $\mathcal{O}(10^5)$, are required to model experimentally observed phenomena. However, accounting for hydrodynamic interactions and Brownian motion are computationally challenging tasks, and even state-of-the-art methods are limited to simulating modest numbers of particles, $\mathcal{O}(10^3)$.

This thesis describes the systematic development and GPU-based implementation of computational methods to perform large scale dynamic simulations of hydrodynamically interacting colloidal particles undergoing Brownian motion. Approximations to the hydrodynamic interactions between particles are built from the periodic fundamental solution for flow at zero Reynolds number and are methodically improved by introducing the multipole expansion and constraints on particle dynamics. Ewald sum splitting, which decomposes the slowly decaying sum of the hydrodynamic interactions into two rapidly decaying sums evaluated independently in real space and Fourier space, is used to accelerate the calculation and serves as the basis for a new technique to rapidly sample the Brownian displacements.

The simulation method is first developed using the ubiquitous low-order Rotne-Prager approximation to the hydrodynamic interactions. Extension of this approximation is achieved *via* the multipole expansion, which introduces the notion of induced force moments whose values are determined from the solution of constraint problems, and methods for handling such constraints are illustrated. The multipole expansion converges slowly when particles are closely separated, a problem which is functionally solved for dynamic simulations by introducing additional constraints on the relative motion of nearly-touching particles through approximations of the lubricating flows between them. Constraints due to lubrication and induced multipoles are combined with a novel, general method to describe constrained hydrodynamic interactions using saddle point matrices. The flexibility of the saddle point approach is demonstrated by straightforward development of a high-accuracy immersed boundary representation of the hydrodynamics within the existing framework. Iterative solution and preconditioning of the constrained hydrodynamic problem is discussed in detail.

Finally, a specific application of the methods developed in this thesis is explored, namely sedimentation in suspensions of attractive (reversibly aggregated) colloidal particles. The simulation results are used to develop a predictive model for the hindered/promoted settling function that describes the mean suspension sedimentation rate as a function of particle concentration and attraction strength, which is shown to be useful in characterizing macromolecular solutions.

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