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Spectral Ewald Acceleration of Stokesian Dynamics for polydisperse suspensions

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ABSTRACT

In this work we develop the Spectral Ewald Accelerated Stokesian Dynamics (SEASD), a novel computational method for dynamic simulations of polydisperse colloidal suspensions with full hydrodynamic interactions. SEASD is based on the framework of Stokesian Dynamics (SD) with extension to compressible solvents, and uses the Spectral Ewald (SE) method [Lindbo and Tornberg (2010) [29]] for the wave-space mobility computation. To meet the performance requirement of dynamic simulations, we use Graphic Processing Units (GPU) to evaluate the suspension mobility, and achieve an order of magnitude speedup compared to a CPU implementation. For further speedup, we develop a novel far-field block-diagonal preconditioner to reduce the far-field evaluations in the iterative solver, and SEASD-nf, a polydisperse extension of the mean-field Brownian approximation of Banchio and Brady (2003) [39]. We extensively discuss implementation and parameter selection strategies in SEASD, and demonstrate the spectral accuracy in the mobility evaluation and the overall $\mathcal{O}(N \log N)$ computation scaling. We present three computational examples to further validate SEASD and SEASD-nf in monodisperse and bidisperse suspensions: the short-time transport properties, the equilibrium osmotic pressure and viscoelastic moduli, and the steady shear Brownian rheology. Our validation results show that the agreement between SEASD and SEASD-nf is satisfactory over a wide range of parameters, and also provide significant insight into the dynamics of polydisperse colloidal suspensions.

1. Introduction

Colloidal suspensions are dispersions of small particles in a viscous solvent, and are found in almost every aspect of our life, ranging from dairy milk to printer ink. They have two distinguishing features: (*i*) Brownian motion of the particles due to thermal fluctuations, and (*ii*) the long-range, non-pairwise–additive hydrodynamic interactions (HIs) mediated by the solvent. As a result of these features, dispersions exhibit many surprising behaviors such as non-Newtonian rheology, glass transitions, phase transitions, *etc.*, and have attracted extensive scientific and engineering interests [1]. Using monodisperse colloidal suspensions as a model system, significant understanding has been achieved through theoretical, simulation, and experimental studies.

However, naturally occurring colloidal suspensions are seldom monodisperse, and particle size differences are often unavoidable. In addition, particle size disparity introduces phenomena otherwise not observed in monodisperse suspensions.

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For example, size polydispersity reduces suspension viscosity [2–4], softens and even melts colloidal glasses [5], and promotes particle segregation in pressure driven flows [6]. Apparently, these behaviors can only be understood by studying dynamics of polydisperse colloidal suspensions.

In this work we develop a computational method based on the framework of Stokesian Dynamics [7] (SD) for fast and realistic dynamic simulations of dense, polydisperse colloidal suspensions, with a focus on suspension rheology. Presently, theoretical and computational studies on polydisperse colloidal suspensions, even for the simplest case of neutrally buoyant hard-sphere particles, are scarce, and heavily focus on the dilute or the short-time limits [8–12]: the former restricts HIs to the two- or three-body level, and the latter ignores suspension dynamic evolution, particularly the influence of Brownian motion. Beyond these limiting cases, we are only aware of the work of Ando & Skolnick [13], who studied particle diffusion in dense polydisperse colloidal suspensions using conventional SD in the context of biological molecular crowding. Their implementation limits HIs to the force–torque level, and therefore is unsuitable for rheological investigations.

A difficulty in dynamic simulations of dense colloidal suspensions is the singular HIs due to the lubrication interactions between close particle pairs. To directly resolve HIs, a computational method must capture the flow details in the small gap between particles. For multipole expansion based methods [7,14,15], a large number of expansion terms are necessary to achieve convergence, and for methods based on surface or spatial discretization, such as the boundary element method [16,17] or direct numerical simulations [18–21], very fine meshing is needed in the gap. Directly resolving lubrication interactions drastically increases the computational cost and limits many studies to low volume fractions. For example, the force coupling method study of Abbas et al. [22] on the dynamics of non-Brownian bidisperse suspensions is limited to particle volume fractions below 20%.

A solution to the above difficulty is the SD framework [7], which exploits the local and pairwise additive nature of lubrication interactions. In SD, the long-range, non-pairwise–additive HIs are computed from the mobility perspective using low-order multipole expansions, and for particles in close contact, lubrication corrections are added pairwise to the corresponding resistance formalism. The corrections are based on the solutions of two-body problems with the far-field contributions removed. In this way, SD avoids directly resolving the singular lubrication interactions. The idea of lubrication correction in SD is general enough for incorporation to other computational methods. For example, similar lubrication corrections has been developed for hydrodynamic multipole methods [14,15,23,24], the force coupling method [25], the lattice Boltzmann method [26], and the fictitious domain method [27]. Moreover, with an appropriate fluid solver, the lubrication corrections can be improved beyond the pairwise level [28]. We feel that, by incorporating the lubrication corrections, many recent computational techniques can significantly extend their accessible parameter range without increasing the computational burden. This point is demonstrated in the present work, which essentially combines the lubrication corrections and the Spectral Ewald (SE) method of Lindbo & Tornberg [29,30] for dynamic simulations of dense polydisperse suspensions.

The Spectral Ewald (SE) method is a new particle mesh technique for computing long-range electrostatic [30] or hydrodynamic [29] interactions, and has recently been incorporated into the boundary integral method for spheroidal particles [31]. Particle mesh techniques including the Particle Mesh Ewald (PME) method [32] and the Smooth Particle Mesh Ewald (SPME) method [33] have been extensively used for calculating HIs with $\mathcal{O}(N \log N)$ computation scaling. Note that, although algorithms based on the fast multipole method [34] can achieve a better computation scaling—down to $\mathcal{O}(N)$—they often have significant computation overheads, and require large system sizes to justify the complexity [35]. Therefore, for many dynamic simulations, the particle mesh techniques remain the practical choice. Notable examples are Accelerated Stokesian Dynamics (ASD) [36] which uses the PME method for the far-field mobility evaluation, and the work of Saintillan et al. [37], where the SPME method is employed to study fiber sedimentation. Compared to other particle mesh techniques, the SE method is spectrally accurate, and can separate errors from the mesh interpolation and the wave-space truncation. Both features are essential for capturing the complicated HIs in polydisperse suspensions.

Another challenge in dynamic simulations of colloidal suspensions is Brownian motion, which is configuration dependent due to the fluctuation–dissipation relation. When Euler–Maruyama time integration is used, the deterministic particle drift due to the Brownian motion must also be included [38]. As a result, computing Brownian-related quantities requires the gradient and the square root of the mobility tensor. Fortunately, these quantities can be evaluated in a matrix-free manner under the framework of ASD, making dynamic studies on hundreds of colloidal particles possible [39,40]. Moreover, the mean-field Brownian approximation, which estimates the mobility tensor based on the near-field HIs, is able to further speed up the computations [39,41]. In this work, these developments are fully incorporated for the dynamic simulation of Brownian polydisperse suspensions. Note that a different approach to treat the Brownian motion is based on fluctuating hydrodynamics [42], where the thermal fluctuations are directly incorporated in the governing fluid equations. It has been applied to the lattice Boltzmann method [43], the force coupling method [44], and the immersed boundary method [45].

The emergence of the General Purpose Graphic Processing Unit (GPGPU) programming often brings significant, sometimes orders of magnitude, speed improvements for many existing algorithms. Recently, Kopp & Höfling [46] implemented the conventional SD for infinite solvent using GPGPU with direct HI summation. Despite the $\mathcal{O}(N^2)$ scaling, they achieved impressive speedup over the CPU implementation. However, to study the dynamics of homogeneous suspensions, further extension to periodic systems are necessary. On the other hand, GPU acceleration of the SPME method [47,48] in molecular dynamics provides access to millisecond-scale dynamics on personal computers. These acceleration techniques are applicable to particle mesh techniques in general, and inspired the present work. In particular, we used GPGPU programming to compute the HIs with the SE method in homogeneous suspensions, and realized almost an order of magnitude speedup in dynamic simulations.