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A fluctuating boundary integral method for Brownian suspensions

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A B S T R A C T

We present a fluctuating boundary integral method (FBIM) for overdamped Brownian Dynamics (BD) of two-dimensional periodic suspensions of rigid particles of complex shape immersed in a Stokes fluid. We develop a novel approach for generating Brownian displacements that arise in response to the thermal fluctuations in the fluid. Our approach relies on a first-kind boundary integral formulation of a mobility problem in which a random surface velocity is prescribed on the particle surface, with zero mean and covariance proportional to the Green's function for Stokes flow (Stokeslet). This approach yields an algorithm that scales linearly in the number of particles for both deterministic and stochastic dynamics, handles particles of complex shape, achieves high order of accuracy, and can be generalized to three dimensions and other boundary conditions. We show that Brownian displacements generated by our method obey the discrete fluctuation–dissipation balance relation (DFDB). Based on a recently-developed Positively Split Ewald method Fiore et al. (2017) [24], near-field contributions to the Brownian displacements are efficiently approximated by iterative methods in real space, while far-field contributions are rapidly generated by fast Fourier-space methods based on fluctuating hydrodynamics. FBIM provides the key ingredient for time integration of the overdamped Langevin equations for Brownian suspensions of rigid particles. We demonstrate that FBIM obeys DFDB by performing equilibrium BD simulations of suspensions of starfish-shaped bodies using a random finite difference temporal integrator.

1. Introduction

Complex fluids containing colloidal particles are ubiquitous in science and industrial applications. Colloidal particles span length scales from several nanometers, such as magnetic nano-propellers [1] and molecular motors [2,3], to a few microns, such as self-phoretic Janus particles [4] and motile microorganisms [5]. In the last decade, increasing attention has been given to the emerging field of *active* colloidal suspensions [6–10], in which particles move autonomously or in response

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to external forces. Despite the advances in the theory and experimental design of passive and active colloids, developing accurate and efficient computational methods that are capable of simulating tens or hundreds of thousands of particles, as well as handling particles of complex shape, still remains a formidable challenge. Here we develop a novel algorithm for generating the Brownian (stochastic) displacements required to perform overdamped Brownian dynamics of a suspension of rigid particles immersed in a Stokes fluid. Our method is based on boundary integral techniques, scales linearly in the number of particles for both deterministic and stochastic dynamics, handles particles of complex shape, and achieves high order accuracy. Because of its close connection to fluctuating hydrodynamics, we refer to our method as the *Fluctuating Boundary Integral Method* (FBIM). We restrict our attention to two-dimensional periodic domains. However, our approach can be extended to three dimensions and confined suspensions.

The two key ingredients that need to be included in a computational method for colloidal suspensions are the long-ranged hydrodynamic interactions (HIs) and the correlated Brownian motion of the particles. In the absence of active and Brownian motion, describing the hydrodynamics of Stokesian suspensions requires the accurate solution of mobility problems [11,12], i.e., computing the linear and angular velocities of the particles in response to applied (external) forces and torques. This process defines the action of a *body mobility matrix*, which converts the applied forces to the resulting particle motions. The mobility matrix encodes the many-body hydrodynamic interactions among the particles, and is therefore dense with long-ranged interactions between *all* bodies. In the presence of Brownian motion, fluctuation–dissipation balance requires the Brownian displacements to have zero mean and covariance proportional to the hydrodynamic mobility matrix. This necessitates an algorithm for generating Gaussian random variables with covariance equal to the body mobility matrix. In this work, we present a new linear-scaling boundary integral method to generate, together, both the deterministic and Brownian displacements.

For passive suspensions of spherical particles in zero Reynolds number flows (infinite Schmidt number), the methods of Brownian [13–17] and Stokesian Dynamics (SD) [18–20] have dominated the chemical engineering community. These methods are tailored to sphere suspensions and utilize a multipole hierarchy truncated at either the monopole (BD) or dipole (SD) level in order to capture the far-field behavior of the hydrodynamic interactions. Modern fast algorithms can apply the action of the truncated mobility matrix with linear-scaling by using the Fast Multipole Method (FMM) for an unbounded domain [17], and using Ewald-like methods for periodic [20,21] and confined domains [15]. The Brownian (stochastic) displacements are typically generated iteratively by a Chebyshev polynomial approximation method [22], or by the Lanczos algorithm for application of the matrix square root [23]. However, since the hydrodynamic interactions among particles decay slowly like the inverse of distance in three dimensions and diverge logarithmically in two dimensions, the condition number of the mobility matrix grows as the number of particles increases (keeping the packing fraction fixed, see [24, Fig. 1]). Therefore, the overall computational scaling for generating Brownian displacements using iterative methods is only superlinear in general.

The fluctuating Lattice Boltzmann (FLB) method has been used for Brownian suspensions for some time [25,26]. This is an explicit solvent method which includes fluid inertia and thus operates at finite Schmidt number instead of in the overdamped limit we are interested in; furthermore, FLB relies on artificial fluid compressibility to avoid solving Poisson problems for the pressure. While the cost of each time step is linear in the number of particles (more precisely, the number of fluid cells) N, in three dimensions $\mathcal{O}\left(N^{2/3}\right)$ time steps are required for vorticity to diffuse throughout the system volume, leading to superlinear $\mathcal{O}\left(N^{5/3}\right)$ overall complexity [24].

As an alternative, methods such as the Fluctuating Immersed Boundary method (FIB) [27] and the fluctuating Force Coupling Method (FCM) [28,29] utilize fluctuating hydrodynamics to generate the Brownian increments in linear time by solving the fluctuating *steady* Stokes equations on a grid. This ensures that the computational cost of Brownian simulation is only marginally larger than the cost of deterministic simulations, in stark contrast to traditional BD approaches. The FIB/FCM approach to generating the Brownian displacements is further improved in the recently-developed Positively Split Ewald (PSE) method [24]. In PSE, the Rotne–Prager–Yamakawa (RPY) tensor [30] is used to capture the long-ranged hydrodynamic interactions, and its action is computed with spectral accuracy by extending the Spectral Ewald [21] method for the RPY tensor. The key idea in PSE is to use the Hasimoto splitting [31] to decompose the RPY tensor into near-field (short-ranged) and far-field (long-ranged) contributions, in a way that ensures that *both* contributions are independently *symmetric positive definite* (SPD). This makes it possible to apply a Lanczos algorithm [23] to generate the near-field contribution with only a small ($\mathcal{O}(1)$) number of iterations, while the far-field contribution is computed by fast Fourier-space methods based on fluctuating hydrodynamics using only a few FFTs. Later in Sec. 3.3, we will apply the same SPD splitting idea to the Green's function of steady Stokes flow to achieve linear scaling in the FBIM.

Essentially all commonly-used methods for overdamped Brownian suspension flows are limited to spherical particles (with some extensions to spheroids [32]), and generalization to include particles of complex shape is generally difficult. Further, these methods employ an *uncontrolled* truncation of a multipole expansion hierarchy and therefore become inaccurate when particles get close to one another as in dense suspensions.

For deterministic Stokes problems, the Boundary Integral Method (BIM) [12] is very well-developed [33–35] and allows one to handle complex particle shapes and achieve *controlled accuracy* even for dense suspensions [36,37]. In the boundary integral framework, the steady Stokes equations are reformulated as an integral equation of unknown densities that are defined on the boundary, using a first-kind (single-layer densities) or second-kind (double-layer densities) formulation, or a mixture of both. Suspended particles of complex geometry can be directly discretized by a surface mesh, and, by a suitable choice of surface quadrature, higher-order (or even spectral) accuracy can be achieved. The key difficulty is handling