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Simulation of concentrated suspensions using the force-coupling method

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ABSTRACT

The force-coupling method (FCM) represents the dynamics of low Reynolds number suspension flows through a distributed, low-order, finite force-multipole expansion and provides an efficient, matrix-free method to solve the mobility problem for the particle motion. In concentrated suspensions, strong short-range lubrication forces are generated between particles in close proximity as fluid in the intervening gap is displaced by the relative motion of the particles. These forces, together with near-surface contact forces, play an important role in the suspension rheology and self-diffusion of particles. However these forces lead to ill-conditioned problems for determining the particle stresses and particle motion in large systems of particles at higher volume fractions. A robust and effective iteration scheme for determining the particle stresslets is described together with a new scheme for including lubrication forces as near-field corrections to the FCM resistance problem. Both the lubrication and far-field interactions are solved as fully coupled systems in $O(N_p \log(N_p))$ operations, for N_p particles, using preconditioned conjugate gradient solvers. Numerical results for particles settling under gravity, particle pairs in linearly varying flows and in concentrated suspensions are compared with previous theoretical results and simulations. Numerical simulations with more than 4000 non-Brownian, spherical particles in a homogeneous shear flow provide results on the pair-distribution function and Lagrangian velocity correlations. The extension of the methods to simulate bidisperse systems or wall-bounded suspensions are discussed.

1. Introduction

Suspensions of small particles in low Reynolds number flows have been the subject of detailed study for several decades. They are relevant to a wide range of engineering and biological applications; materials processing, particle coating, microdevices for particle separation or mixing, waste treatment, blood flow and cell adhesion, to name a few. Concentrated suspensions are characterized by both the long-range multi-body hydrodynamic interactions of particles and the short-range viscous lubrication forces that act between particles near to contact. For example, the volume fraction of red blood cell in human blood flow is typically ~45% [1]. Even in nominally dilute suspensions, both long-range flow interactions and short-range lubrication forces are important for particles in microfluidic devices where particles are confined by flow geometry [2,3].

Numerical simulations of monodisperse suspension flows in uniform shear have had a large impact on the characterization and modeling of low Reynolds number suspensions. The principal tools have been Stokesian Dy-namics (SD) [4], multipole expansions [5–7], and boundary integral methods [8]. Lattice-Boltzmann methods (LBM) bridge both finite Reynolds number and low Reynolds number systems and have also contributed [9,10]. The force-coupling method (FCM) [11,12] and subsequent

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developments, bridge both Stokes flows and finite, low Reynolds number systems. FCM may be used to simulate large systems of particles in both open and wall-bounded flows in fully three-dimensional configurations.

For the accurate simulation of Stokes flow, a numerical method should be able to capture both the long-range multi-body interactions and the short-range lubrication interactions. Especially, the singular nature of the lubrication forces hinders the development of numerical schemes. For example, the most straightforward and exact numerical method would be the direct numerical simulation with an arbitrary Lagrangian–Eulerian technique [13,14]. However, considering that the lubrication forces for the normal and tangential motions between a particle pair are, respectively, $\sim 1/\epsilon$ and $\log\epsilon$, in which $a\epsilon$ denotes the separation distance between two particles and a is the particle radius, the grid spacing should be smaller than at least $10^{-3}a$—$10^{-4}a$ to resolve the lubrication forces. Correspondingly, the time step size also should be very small, of the order of 10^{-3}—10^{-4}, making long-term simulations of the suspension dynamics too costly.

In Stokes flow, the hydrodynamic interactions are determined solely by the instantaneous configuration of particles. Using the special properties of Stokes flow, several numerical methods have been developed focusing on computing hydrodynamic interactions rather than resolving the whole flow field. The multipole expansion is a representative approach to consider the hydrodynamic interactions between particles. However, Cichocki and Felderhof [5] reported that the number of multipole moments needed to resolve the hydrodynamic interaction becomes impractically large as the gap between particles becomes so small that the lubrication force plays an important role. Durlofsky et al. [15] developed the Stokesian Dynamics method, which is a low-order multipole representation, supplemented by short-range lubrication forces, to compute the position and movement of suspended particles. In the Stokesian Dynamics, they assumed the lubrication interaction can be added in a pair-wise manner in the resistance formulation, which has become a standard approach for incorporating the lubrication forces [6,9,16]. Sierou and Brady [17] developed the Accelerated Stokesian Dynamics (ASD) method and performed the simulations of up to 1000 particles [18].

The boundary element method (BEM) is another distinguishing numerical method for Stokes flows, see for example [8]. BEM can calculate the hydrodynamic interactions in particulate suspensions with greater accuracy. However, even here some form of lubrication or contact forces must be included between rigid particles. Ingber et al. [19] have developed a traction-corrected BEM which can accurately calculate the lubrication interaction. Although BEM can simulate wall-bounded suspensions and suspension of particles with arbitrary shapes [20,21], due to the high computational cost most simulations are done in 2-dimensions or with relatively small numbers of particles.

Since Nguyen and Ladd [9] implemented the lubrication interaction into the lattice-Boltzmann simulation, LBM has become popular for the suspensions in the low to finite Reynolds number flows [10,22,23]. Compared to SD, LBM is computationally inexpensive and a rigid wall boundary can be included without any special treatment, while present techniques for SD use an image method [24,25] or wall particles [26,27] to represent a rigid wall.

Maxey and Patel [11] developed the force-coupling method (FCM) for Stokes flow by replacing the Dirac delta function in the standard multipole expansion [28] by a localized force envelope. The force-coupling method has been verified [29,12,30] and applied in many suspension flows; for example, a sedimentation problem [31], bimodal suspensions [32], turbulent flows [33], and biological flows [34]. Since multi-body hydrodynamic interactions are accounted for by solving the Stokes equation, the computational cost of FCM depends on the choice of the Stokes solver. In a periodic domain, the long-range hydrodynamic interactions can be calculated in $O(N_p log N_p)$ operations using a Fourier spectral method, in which N_p is the number of particles. Dance and Maxey [31] performed the numerical simulations of particle sedimentation with up to 10,000 particles. The force-coupling method can be implemented with any existing flow solver by adding functions to integrate and project the force envelope. Recently, Liu et al. [35] showed that the force-coupling method can simulate suspensions of ellipsoidal particles by appropriately rescaling the force envelopes.

In the force-coupling method, the translational and angular velocities of a particle are estimated by the local average of the fluid velocity weighted by the corresponding force envelopes. This approach has a computational advantage by reducing the number of grid points necessary to resolve a particle. Once the resolution is fine enough to resolve the force envelope, FCM can accurately reproduce the far-field solution. Typically, it requires only $a/\Delta x \simeq 3$ to resolve a particle in which Δx is the grid spacing. This is less than other methods, such as the immersed boundary method or the lattice-Boltzmann simulations. On the other hand, it has a disadvantage that the near-field solution is not correctly resolved. When two particles are close, the force-coupling method cannot reproduce the lubrication effects [12]. As a result, the force-coupling method has been used mainly for low volume fractions, $\phi < 0.1$.

Dance and Maxey [36] developed a method to incorporate the lubrication effects into the force-coupling method based on the exact solution of the viscous lubrication interactions of a particle–pair. They employed a predictor–corrector type approach. First, the far-field interaction is calculated by the standard FCM to estimate the lubrication force and then the lubrication force is used as a feedback force in the mobility formulation. By construction, their method can reproduce the exact particle velocities for a particle–pair interaction. At low volume fractions in which most lubrication interactions are from particle doublets, the 'lubrication barrier' would be sufficient [32]. However, it is not straightforward how to generalize the approach to include multi-body interactions, which generally requires the addition of lubrication interactions to a resistance formulation [15].

The main goal of this paper is to develop an efficient method to incorporate the lubrication forces for general volume fractions into the force-coupling method. The lubrication correction method developed in this paper can be easily extended to the bidisperse suspensions or the wall-bounded flows [37].