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An integral equation formulation for rigid bodies in Stokes flow in three dimensions

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ABSTRACT

We present a new derivation of a boundary integral equation (BIE) for simulating the three-dimensional dynamics of arbitrarily-shaped rigid particles of genus zero immersed in a Stokes fluid, on which are prescribed forces and torques. Our method is based on a single-layer representation and leads to a simple second-kind integral equation. It avoids the use of auxiliary sources within each particle that play a role in some classical formulations. We use a spectrally accurate quadrature scheme to evaluate the corresponding layer potentials, so that only a small number of spatial discretization points per particle are required. The resulting discrete sums are computed in $\mathcal{O}(n)$ time, where n denotes the number of particles, using the fast multipole method (FMM). The particle positions and orientations are updated by a high-order time-stepping scheme. We illustrate the accuracy, conditioning and scaling of our solvers with several numerical examples.

1. Introduction

In viscous flows, the mobility problem consists of computing the translational and rotational velocities $(\boldsymbol{v}_i, \boldsymbol{\omega}_i)$ induced on a collection of n rigid bodies when prescribed forces and torques $(\boldsymbol{F}_i, \boldsymbol{T}_i)$ are specified on each one. The Stokes equations, which are linear, govern the ambient viscous fluid at vanishing Reynolds number limit. Thereby, there exists a well-defined *mobility matrix* denoted by M such that

$$\boldsymbol{V} = M\boldsymbol{F}, \tag{1.1}$$

where $\boldsymbol{V} = (\boldsymbol{v}_1, \boldsymbol{\omega}_1, \ldots, \boldsymbol{v}_n, \boldsymbol{\omega}_n)$ and $\boldsymbol{F} = (\boldsymbol{F}_1, \boldsymbol{T}_1, \ldots, \boldsymbol{F}_n, \boldsymbol{T}_n)$.

Reformulating the problem as an integral equation has several advantages over direct discretization of the governing partial differential equations themselves. First, integral equation methods require discretization of the particle boundaries alone, which leads to an immediate reduction in the size of the discretized linear system. Equally important, carefully chosen integral representations result in well-conditioned linear systems, while discretizing the Stokes equations directly leads to highly ill-conditioned systems. Moreover, the integral representation can be chosen to satisfy the far field boundary conditions necessary to model an open system, thereby eliminating the need for artificial truncation of the computational domain. Lastly, combining high-order quadrature methods and suitable fast algorithms, boundary integral equations for complex geometries can be solved to high accuracy in optimal or near optimal time [7,15,24,29,41].

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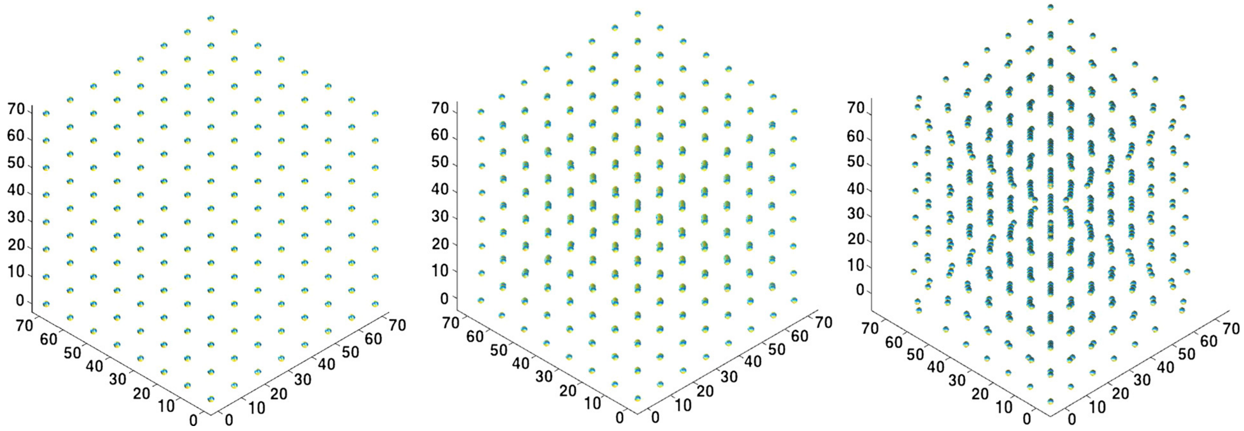

Fig. 1. Self-assembly of chains in a magnetorheological fluid. Snapshots from a simulation of a cubic lattice of 512 paramagnetic spheres subjected to a uniform magnetic field $\boldsymbol{H}_0$ in a Stokesian flow. We use spherical harmonic expansions of degree $p = 8$ to represent functions on each sphere, requiring a total of 294912 degrees-of-freedom per time-step to compute hydrodynamic and magnetic interactions. At each time-step, a magnetostatic problem is solved for the current particle configuration; the Maxwell stresses thus obtained at the particle boundaries give rise to a mobility problem (details in Section 4). Our BIE formulations for both the fluid velocity and magnetic potential problems lead to well-conditioned linear systems. Summation of far-field interactions is accelerated via Stokes and Laplace FMMs [13]. On an average, this simulation took 5 minutes per time-step on a single node with Intel Xeon E–2690 v2 (3.0 GHz) processor and 24 GB of RAM.

A variety of integral representations for the mobility problem have been introduced, often in the form of first kind integral equations [10] or second kind integral equations with n additional unknowns and an equal number of additional constraints [23]. While these have been shown to be very effective, it is advantageous (when n is large and the rigid bodies have complicated shape) to work with well-conditioned second kind boundary integral formulations which are free of additional constraints. Such schemes have been developed earlier [18], using the Lorentz reciprocal identity. The equation which we derive below in Section 2 is essentially the same, but obtained using a different principle—namely that the interior of a rigid body must be stress free. The mobility problem can also be solved using a double layer representation that doesn't involve additional unknowns. For a detailed discussion of the latter approach, we refer the reader to [1,32]. Our formulation has the advantage that certain derivative quantities, such as fluid stresses, can be computed using integral operators with weakly singular kernels instead of hypersingular ones, simplifying the quadrature issues.

Based on this formulation, we present a numerical algorithm in Section 3 to solve the mobility problem and evolve the position and orientation of the rigid bodies. In Section 4, we discuss several applications and present results from our numerical experiments (a sample simulation with large n is depicted in Fig. 1).

2. The mobility problem

Let $\{D_i\}_{i=1}^n$ be a set of n disjoint rigid bodies in $\mathbb{R}^3$ with boundaries Γ_i. Let $\boldsymbol{F}_i, \boldsymbol{T}_i$ denote the force and torque exerted on D_i, let $\boldsymbol{v}_i, \boldsymbol{\omega}_i$ denote the translational and rotational velocity of D_i, and let $\boldsymbol{x}_i^c$ denote the centroid of Γ_i. Let E be the domain exterior to all of the rigid bodies $\{D_i\}$, and assume that the fluid in E is governed by Stokes flow with viscosity $\mu = 1$. For a given velocity field $\boldsymbol{u}(\boldsymbol{x}) \in \mathbb{R}^3$ at a point $\boldsymbol{x} \in E$, we denote the corresponding fluid pressure, strain and stress tensors by p, $e(\boldsymbol{u})$ and σ, respectively. On the surface of the rigid bodies, $\boldsymbol{f} = \sigma \cdot \boldsymbol{n}$ denotes the surface force or surface traction exerted by the fluid on the rigid body D_i. For the sake of simplicity, we assume there are no volume forces. The governing equations for the mobility problem are then given by:

$$-\Delta \boldsymbol{u} + \nabla p = \boldsymbol{0}, \quad \nabla \cdot \boldsymbol{u} = 0 \;\; \forall \boldsymbol{x} \in E, \tag{2.1}$$

$$\boldsymbol{u}(\boldsymbol{x}) = \boldsymbol{v}_i + \boldsymbol{\omega}_i \times (\boldsymbol{x} - \boldsymbol{x}_i^c) \;\; \forall \boldsymbol{x} \in \Gamma_i, \tag{2.2}$$

$$\int_{\Gamma_i} \boldsymbol{f}\, dS_y = \int_{\Gamma_i} \sigma \cdot \boldsymbol{n}\, dS_y = -\boldsymbol{F}_i, \quad \int_{\Gamma_i} (\boldsymbol{x} - \boldsymbol{x}_i^c) \times \boldsymbol{f}\, dS_y = -\boldsymbol{T}_i, \tag{2.3}$$

$$\boldsymbol{u}(\boldsymbol{x}) \to \boldsymbol{0} \;\text{ as }\; |\boldsymbol{x}| \to \infty. \tag{2.4}$$

It should be noted that the forces and torques, $\boldsymbol{F}_i$, and $\boldsymbol{T}_i$ are *known* and the translational and rotational velocities $\boldsymbol{v}_i$, and $\boldsymbol{\omega}_i$ are *unknown*.

Before turning to the integral equation, however, we state and prove a simple uniqueness result. To prove uniqueness, we need the following lemma contained in [32]: