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Benchmark solutions

Mobilities of polydisperse hard spheres near a no-slip wall

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ABSTRACT

We have derived an analytical formulation for far-field hydrodynamic interactions among unequal size hard spheres near a no-slip wall and have implemented the formulation in a Stokesian dynamics model to simulate a suspension of polydisperse particles in a semi-bounded domain. The formulation is based on the multipole expansion of the boundary integral of Stokes flow, and the mobility tensors are deduced from Fáxen's law together with Green's function for Stokes flow near a no-slip wall. Lubrication approximation is incorporated to account for the close-distance interactions between any two particles and also between the particles and the wall. The implementation is validated against previous formulations for equal size particles and against a boundary-element code for unequal size particles. The code can be used to simulate the Stokesian or Brownian interaction of unequal particles in presence of a no-slip wall. In the current study, we applied the Stokesian dynamics model to investigate the trajectories of two unequal hard spheres and their redistribution during sedimentation parallel to a wall. We further used it to demonstrate the cases of many-particle sedimentation toward or parallel to a wall.

1. Introduction

Hydrodynamic interactions near a solid surface between particles in a particulate suspension play a vital role in many physical and technological processes. Examples include locomotion of microorganisms near surfaces [1–4], microfluidic devices [5], oil recovery [6,7], water and waste treatment [8], and energy storages [9]. In the limit of Stokes flow, theoretical models have long been established to account for particle-particle pair interaction in free space, including long-range or far-field interaction [10], close-range lubrication [11], unequal particle sizes [12], and surface slip effect [13] (here "far-field" refers to the situation where particles are outside of each other's lubrication region, rather than a location far away from the particles as defined in certain cases [14,15]). Although the spherical approximation was mostly often used in theoretical studies, non-spherical shapes were also considered, e.g., ellipsoidal [16] or even arbitrary shape in some cases [17]. In those models, the particle interactions are usually described in terms of the mobility tensors that represent the motion of the particles under specified external forces, or in terms of the resistance tensors that represent the hydrodynamic resistance for given particle motion. Based on the theoretical descriptions of spherical shape, the Stokesian dynamics method was developed to simulate interactions of many particles suspended in a flow [18]. In the Stokesian dynamics method, the grand mobility matrix is first built that accounts for the far-field interaction of any two particles; then lubrication is introduced for any particle pair whose separation distance is within a prescribed threshold. The lubrication effect between two closely located particles is written in the form of the resistance tensor, and after subtracting the far-field resistance to avoid double counting, its inverse is added to the grand mobility matrix to represent the corrected mobility. Stokesian dynamics can accurately account for both long-range and short-range hydrodynamic interactions, and on the other hand, it is extremely efficient as compared with computational fluid dynamics (CFD) methods when many particles are involved. Thus, Stokesian dynamics is a popular approach for simulating colloids and suspensions.

In real applications, particulate flows are usually bounded by a solid surface, and near-surface interactions can be an important part in the overall flow behavior. Thus, developing corresponding theoretical models for hydrodynamics of colloidal particles near a wall has also been a point of interest for several decades [19–21]. Former developments include the interaction of individual particles with a wall at far field [22,23], lubrication limit [24], as well as in the presence of surface slip [25]. Since initial introduction of Stokesian dynamics, several researchers have focused on the study of dynamics of particles in bounded domains. Brady and Durlofsky [26] considered the effect of the wall on energy dissipation by incorporating an integral model of wall patches. In a later work,

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Nott and Brady [27] discretized the wall using a chain of fixed particles placed close to each other. The fixed-particle implementation of the wall effect is straightforward and can predict the qualitative behavior of the particles; however, due to the leaking effect and a non-smooth surface, such a wall model is not accurate. Some others [28,29] have used multipole expansion of the hydrodynamic force densities and an image representation to account for the presence of a wall. Swan and Brady constructed the mobility tensors for hydrodynamic interaction of equal-size particles directly from the Faxén law [22]. More recently, some studies have derived mobilities of hard spheres bounded by non-flat surfaces, e.g., cylinders [30–32] and spherical cavities [33,34].

When a flat wall is considered, previous formulations are limited to spherical particles of equal size interacting with one other, and the formulation of two near-wall particles with different sizes is still not readily available. Such formulation would be useful for developing Stokesian dynamics simulations of more general situations that are encountered in many applications and is therefore the goal of the present study. In addition to the theoretical derivation and its validation, we will also apply the formulation to the cases of two particles, as well as many particles, sedimenting near a wall.

The closest reference to our study is that of Swan and Brady [22], who has derived the mobility tensors for two equal size spheres near a no-slip wall. In this paper, we will follow their approach to derive the mobility tensors for two particles of unequal sizes; then, we will implement these tensors in a Stokesian dynamics model and test its validity against numerical simulations of a boundary-element method. These mobility tensors are given explicitly here in this work, and a C++ code computing them will be available upon request.

2. Theoretical formulations

2.1. The derivation procedure

For a specific configuration of N particles, its hydrodynamics is governed by a linear equation system. That is, a grand mobility matrix, $\mathcal{M}$, describes how the translational, rotational, and strain disturbance of the particles relate to the total force, torque, and stresslet on the particles [18,26] according to

$$\begin{pmatrix} \mathbf{U}^\alpha - \mathbf{U}^\infty(\mathbf{x}^\alpha) \\ \mathbf{U}^\beta - \mathbf{U}^\infty(\mathbf{x}^\beta) \\ \vdots \\ \boldsymbol{\Omega}^\alpha - \boldsymbol{\Omega}^\infty(\mathbf{x}^\alpha) \\ \boldsymbol{\Omega}^\beta - \boldsymbol{\Omega}^\infty(\mathbf{x}^\beta) \\ \vdots \\ -\mathbf{E}^\infty(\mathbf{x}^\alpha) \\ -\mathbf{E}^\infty(\mathbf{x}^\beta) \\ \vdots \end{pmatrix} = \begin{pmatrix} \mathbf{M}^{\alpha\alpha}_{\mathrm{UF}} & \mathbf{M}^{\alpha\beta}_{\mathrm{UF}} & \cdots & \mathbf{M}^{\alpha\alpha}_{\mathrm{UL}} & \mathbf{M}^{\alpha\beta}_{\mathrm{UL}} & \cdots & \mathbf{M}^{\alpha\alpha}_{\mathrm{US}} & \mathbf{M}^{\alpha\beta}_{\mathrm{US}} & \cdots \\ \mathbf{M}^{\beta\alpha}_{\mathrm{UF}} & \mathbf{M}^{\beta\beta}_{\mathrm{UF}} & \cdots & \mathbf{M}^{\beta\alpha}_{\mathrm{UL}} & \mathbf{M}^{\beta\beta}_{\mathrm{UL}} & \cdots & \mathbf{M}^{\beta\alpha}_{\mathrm{US}} & \mathbf{M}^{\beta\beta}_{\mathrm{US}} & \cdots \\ \vdots & \vdots & & \vdots & \vdots & & \vdots & \vdots & \\ \mathbf{M}^{\alpha\alpha}_{\Omega\mathrm{F}} & \mathbf{M}^{\alpha\beta}_{\Omega\mathrm{F}} & \cdots & \mathbf{M}^{\alpha\alpha}_{\Omega\mathrm{L}} & \mathbf{M}^{\alpha\beta}_{\Omega\mathrm{L}} & \cdots & \mathbf{M}^{\alpha\alpha}_{\Omega\mathrm{S}} & \mathbf{M}^{\alpha\beta}_{\Omega\mathrm{S}} & \cdots \\ \mathbf{M}^{\beta\alpha}_{\Omega\mathrm{F}} & \mathbf{M}^{\beta\beta}_{\Omega\mathrm{F}} & \cdots & \mathbf{M}^{\beta\alpha}_{\Omega\mathrm{L}} & \mathbf{M}^{\beta\beta}_{\Omega\mathrm{L}} & \cdots & \mathbf{M}^{\beta\alpha}_{\Omega\mathrm{S}} & \mathbf{M}^{\beta\beta}_{\Omega\mathrm{S}} & \cdots \\ \vdots & \vdots & & \vdots & \vdots & & \vdots & \vdots & \\ \mathbf{M}^{\alpha\alpha}_{\mathrm{EF}} & \mathbf{M}^{\alpha\beta}_{\mathrm{EF}} & \cdots & \mathbf{M}^{\alpha\alpha}_{\mathrm{EL}} & \mathbf{M}^{\alpha\beta}_{\mathrm{EL}} & \cdots & \mathbf{M}^{\alpha\alpha}_{\mathrm{ES}} & \mathbf{M}^{\alpha\beta}_{\mathrm{ES}} & \cdots \\ \mathbf{M}^{\beta\alpha}_{\mathrm{EF}} & \mathbf{M}^{\beta\beta}_{\mathrm{EF}} & \cdots & \mathbf{M}^{\beta\alpha}_{\mathrm{EL}} & \mathbf{M}^{\beta\beta}_{\mathrm{EL}} & \cdots & \mathbf{M}^{\beta\alpha}_{\mathrm{ES}} & \mathbf{M}^{\beta\beta}_{\mathrm{ES}} & \cdots \\ \vdots & \vdots & & \vdots & \vdots & & \vdots & \vdots & \end{pmatrix} \cdot \begin{pmatrix} \mathbf{F}^\alpha \\ \mathbf{F}^\beta \\ \vdots \\ \mathbf{L}^\alpha \\ \mathbf{L}^\beta \\ \vdots \\ \mathbf{S}^\alpha \\ \mathbf{S}^\beta \\ \vdots \end{pmatrix}, \tag{1}$$

where superscripts α and β are particle labels, $\mathbf{U}$ and $\boldsymbol{\Omega}$ are respectively the translational and rotational velocities of a particle, $\mathbf{U}^\infty$, $\boldsymbol{\Omega}^\infty$, and $\mathbf{E}^\infty$ are respectively the far-field velocity, vorticity, and strain rate imposed at the center of the particle, **F, L**, and **S** are respectively the total external force, torque, and stresslet on the particle, and matrix blocks such as $\mathbf{M}_{\mathrm{UF}}$ are the mobility tensors in the grand mobility matrix $\mathcal{M}$. Each mobility tensor expresses the relationship between **U, Ω**, or **E** and **F, L**, or **S** as indicated by the its subscripts. The superscripts indicate either self mobility, e.g., $\alpha\alpha$ for the effect of particle α on itself, or mutual mobility, e.g., $\alpha\beta$, for the effect of particle β on particle α.

To derive the mobility tensors in Eq. (1) that involves the presence of a wall, we follow a previously established approach [22,26] for Stokesian dynamics. Starting from the boundary-integral equation of Stokes flow by Ladyzhaneskaya [35], the disturbance velocity at every point in a flow domain is related to the surface integral of force traction distribution function through Green's function [36]. When a cluster of N rigid spherical particles is considered, the boundary-integral equation can be approximated by a multipole expansion of the integrals about each particle's center. That is, the velocity field due to the presence of the particles is related to the force, torque, and stresslet on each particle by [18,26]

$$\begin{aligned} u_i(\mathbf{x}) - U^\infty(\mathbf{x}) = \frac{1}{8\pi\eta}\sum_{\beta=1}^{N}\Bigg\{\Bigg[\left(1+\frac{a_\beta^2}{6}\nabla_{\mathbf{y}}^2\right)G_{ij}F_j^\beta\Bigg] \\ + \frac{1}{2}\epsilon_{jkl}\frac{\partial}{\partial y_k}G_{il}L_j^\beta \\ + \frac{1}{2}\left(1+\frac{a_\beta^2}{10}\nabla^2\right)\left(\frac{\partial}{\partial y_k}G_{ij}+\frac{\partial}{\partial y_j}G_{ik}\right)S_{jk}^\beta\Bigg\}\Bigg|_{\mathbf{y}=\mathbf{x}^\beta}, \end{aligned} \tag{2}$$

where $i, j, k = 1, 2, 3$ represent Cartesian coordinates, η is the fluid viscosity, a_β is the radius of particle β, ϵ_{ijk} is the permutation tensor, and $G_{ij}(\mathbf{x},\ \mathbf{y})$, or $\mathbf{G}(\mathbf{x}, \mathbf{y})$, is Green's function for Stokes flow, which will be discussed next. Furthermore, $F_j^\beta = -\int_\beta f_i\, dA = -\int_\beta \tau_{ji}n_i\, dA$ is a component of the total force **F** on particle β, n_j represents the surface normal pointing into the fluid, $L_j^\beta = -\int_\beta \epsilon_{ijk}(x_j - x_j^\beta) f_k\, dA$ is a component of the total torque **L**, S_{jk}^β is a component of the stresslet **S** and has the form of

$$S_{ij}^\beta = -\frac{1}{2}\int_\beta \left[\left(x_i - x_i^\beta\right)f_j + f_i(x_j - x_j^\beta) - \frac{2}{3}\delta_{ij}(x_k - x_k^\beta)f_k\right] dA. \tag{3}$$

Note that in Eq. (2), higher order terms in the multipole expansion of Ladyzhaneskaya's boundary integral equation [35] have been truncated off.

Since a semi-bounded flow is considered in the present study, Green's function for Stokes flow near a wall will be used in Eq. (2). This function is a superposition of a Stokeslet at the source point location in an unbounded domain, i.e., the free-space Green's function, $\mathbf{G}^{fs}$, and its image about the wall, $\mathbf{G}^w(\mathbf{x},\ \mathbf{y},\ h)$. That is, $\mathbf{G}(\mathbf{x}, \mathbf{y}, h) = \mathbf{G}^{fs}(\mathbf{x}, \mathbf{y}) + \mathbf{G}^w(\mathbf{x}, \mathbf{y}, h)$, where $\mathbf{x}$ and $\mathbf{y}$ are the field point and source point, respectively, and h is the distance of the source point from the wall [36]. The wall normal is in the positive direc-