

Methods paper for rigid bodies

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Abstract

We consider suspensions of rigid bodies in two dimensions ...

Keywords: Stokes flow, Boundary integral method, Rigid body suspensions

1. Introduction

Bryan will write this section

This is a methods paper

- Boundary integral equation formulation
- STIV
- FMM
- Near-singular integration
- Pressure and energy dissipation calculations
- Time integrator

2. Formulation

2.1. Problem Formulation

We will consider a collection of particles in a planar (two dimensional) flow. The fluid will be in a domain Ω with a boundary $\partial\Omega$. The boundary $\partial\Omega$ is the union of the surfaces of N suspended particles each with a boundary Γ_k , $1 \leq k \leq N$, the surfaces of M solid walls each with boundary, Γ_ℓ $N+1 \leq \ell \leq N+M$ and optionally a containing wall denoted Γ_0 . The suspended particles are all rigid and at each time step we will solve for their translational velocity \mathbf{u}_k^T and angular velocity ω_k , allowing us to update their centers and orientations, \mathbf{c}_k and θ_k respectively. Particles and interior walls will be undergoing a net force $\mathbf{F}_{k/\ell}$ and torque $L_{k/\ell}$.

2.2. Repulsion Forces

It is well known that the exact solutions of the Stokes equations prohibit contact between particles in finite time due to lubrication forces. In theory therefore if we solve the Stokes equations accurately enough contact will be avoided. Achieving this level of accuracy however could require a prohibitively fine mesh or small time step size, in particular for dense suspensions. In order to keep computational costs reasonable we must turn to alternative approaches.

One such approach is to introduce an artificial repulsion force. There are many possible choices for the type of force. One possibility is a Leonard-Jones type force that grows exponentially as two particles become close together (need citations). This has been shown to work for dense suspensions, however the resulting

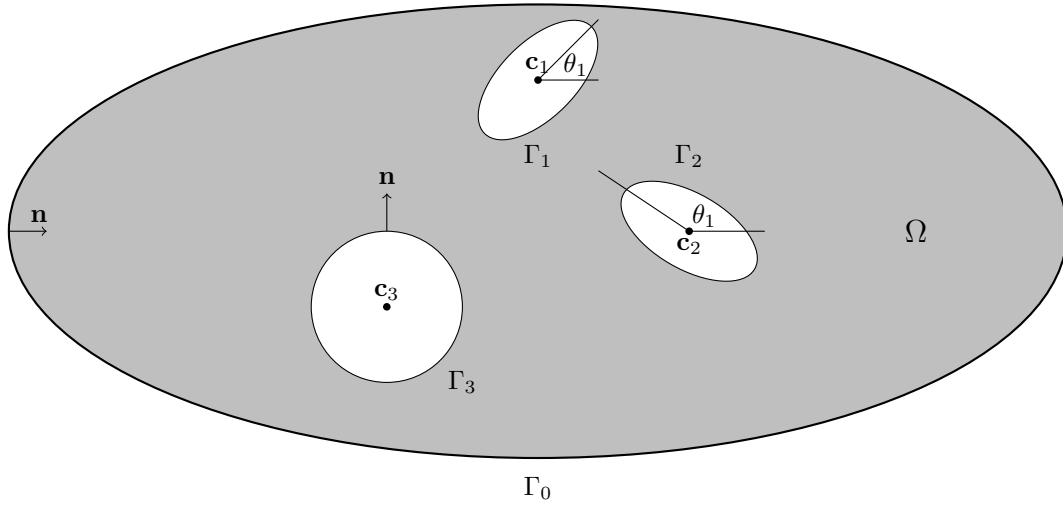


Figure 1: Sketch of a possible domain Ω . Γ_1 and Γ_2 enclose particles, while Γ_3 encloses a solid wall. The outer boundary Γ_0 need not be present. The boundary $\partial\Omega$ is $\Gamma_0 \cup \bigcup_{i=1}^{N+M} \Gamma_i$. The vector \mathbf{n} is the unit normal vector pointing into the fluid domain.

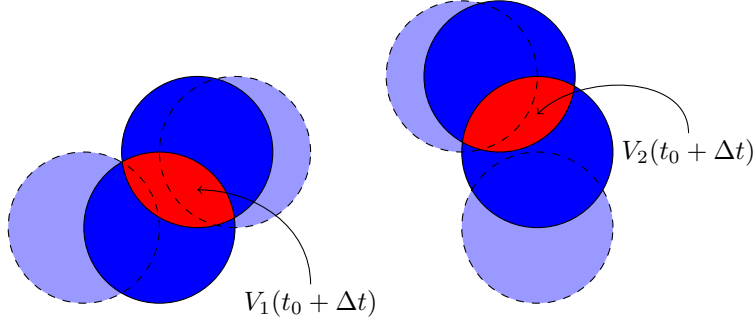


Figure 2: Sketch of potential collisions.

ODEs become very stiff as the separation between particles decreases, thus requiring smaller time steps. In addition this type of force does not guarantee no collisions. If the time step is too large collisions can still occur. An alternative approach is to choose the forces in such a way as to explicitly guarantee each time step is collision free.

The main algorithm will proceed as follows. At each time step t^n the Stokes equations are solved and the particles are advanced to a candidate configuration at t^{n+1} . At this point we can check for collisions. If no collisions are found, the candidate configuration is accepted, otherwise it is rejected and we resolve the Stokes equations at t^n with an artificial repulsion force, adjusting this force as necessary until the candidate configuration at time t^{n+1} is collision free and can be accepted. The remainder of this section is dedicated to describing how this artificial repulsion force is computed.

2.3. Contact definition

Before any discussion of resolving collisions we must define a metric that measures collisions. This metric will keep track of all possible pairwise collisions. If an entry of $\mathbf{V}(t)$ is less than 0 at a time t , then a collision has occurred and a repulsion force must be added. There are several possible choices for $\mathbf{V}(t)$, the simplest of which is simply a signed distance between all points on all particles. We will use the concept of *Space-Time*

Interference Volumes (STIV) introduced by Harmon et al.[2] and adapted for suspension modeling by Lu et al.[5].

Given a particle configuration $S(t)$ for which $S(t_0)$ is collision-free, for each point $\mathbf{X}(s, t)$ on $S(t)$ we define $\tau_I(s)$, $t_0 < \tau_I \leq t$ to be the first instance for which \mathbf{X} comes into contact with a different point on $S(t)$. The STIV for the time interval $[t_0, t]$ is

$$V(S, t) = - \int_{S(t_0)} \int_{\tau_I(s)}^t \sqrt{\epsilon^2 + (\mathbf{u}(s, \tau) \cdot \mathbf{n}(s, \tau))^2} d\tau ds,$$

where the constant ϵ is a smoothing parameter. The time integral in this expression ensures that no contact is missed even if one particle passes completely through another (or through a solid wall) in a single time step. This allows us to take large time steps and not be worried about missing collisions. $\mathbf{V}(S, t)$ can be interpreted as the area of the surface with coordinate $(\mathbf{X}(s, \tau), \epsilon\tau)$ for all (s, τ) such that $\tau_I(s) \leq t$.

In [5] an infinitesimal version of the STIV is derived. Starting from a collision-free configuration at t_0 , for a fixed τ the set of points s such that $\tau_I(s) \leq \tau$ is the contact area. This area is a set of boundary segments. For one such segment we can let $s_1(\tau)$ and $s_2(\tau)$ be the extents of contact at time τ .

$$\mathbf{V}(\mathbf{u}, t) = - \int_{s_1(t)}^{s_2(t)} \sqrt{\epsilon^2 + (\mathbf{u}(s, t) \cdot \mathbf{n}(s, t))^2} ds + \epsilon,$$

along with the variation,

$$d_{\mathbf{u}} V[\delta \mathbf{u}] = - \int_{s_1(t)}^{s_2(t)} \frac{(\mathbf{n} \cdot \mathbf{u})(\mathbf{n} \cdot \delta \mathbf{u})}{\sqrt{\epsilon^2 + (\mathbf{u} \cdot \mathbf{n})^2}} ds.$$

2.4. Governing Equations

The governing equations for this problem are the incompressible Stokes equations,

$$-\mu \Delta \mathbf{u} + \nabla p = \mathbf{f} \text{ in } \Omega, \tag{1a}$$

$$\nabla \cdot \mathbf{u} = 0 \text{ in } \Omega, \tag{1b}$$

where $\mathbf{u}(\mathbf{x})$ is the fluid velocity, $p(\mathbf{x})$ is the fluid pressure, $\mathbf{f}(\mathbf{x})$ are body forces acting on the fluid and μ is the dynamic viscosity of the fluid. For simplicity we will take μ to be 1 for the remainder of this paper. We will assume Dirichlet boundary conditions on the velocity,

$$\mathbf{u} = \mathbf{u}_b \text{ on } \partial\Omega, \tag{2}$$

subject to the constraint

$$\int_{\Gamma_i} \mathbf{u}_b \cdot \mathbf{n} ds = 0, \quad 0 \leq i \leq N + M, \tag{3}$$

which is necessary for global conservation of mass and does not allow for sources or sinks.

The incompressible Stokes equations can be restated as a minimization problem. Consider the functional,

$$\mathcal{J}(\mathbf{u}) = \int_{\Omega} \nabla \mathbf{u} : \nabla \mathbf{u} - 2\mathbf{f} \cdot \mathbf{u} d\Omega,$$

and the associated constrained minimization problem,

$$\min \mathcal{J}(\mathbf{u}) : \nabla \cdot \mathbf{u} = 0 \text{ in } \Omega.$$

Introducing p , a Lagrange multiplier for the incompressibility condition, we can construct a Lagrangian for this system,

$$\mathcal{L}(\mathbf{u}, p) = \mathcal{J}(\mathbf{u}) - \int_{\Omega} 2p \nabla \cdot \mathbf{u} \, d\Omega. \quad (4)$$

First order optimality (KKT) conditions for $\mathcal{L}(\mathbf{u}, p)$ recover the incompressible Stokes equations. For our problem, in addition to the incompressibility condition, we wish to enforce the constraint that the solution \mathbf{u} at a time t_0 should not introduce collisions at time $t_0 + \Delta t$, in other words $\mathbf{V}(t_0 + \Delta t) \geq \mathbf{0}$. This constraint can be incorporated in the Lagrangian (4) with the introduction of a Lagrange multiplier $\boldsymbol{\lambda}$ with one component for each possible collision volume,

$$\tilde{\mathcal{L}}(\mathbf{u}, p, \boldsymbol{\lambda}) = \mathcal{L}(\mathbf{u}, p) + \boldsymbol{\lambda} \cdot \mathbf{V}(t_0 + \Delta t). \quad (5)$$

First order optimality for (5) yields the Stokes equations with a modified forcing function,

$$-\Delta \mathbf{u} + \nabla p = \mathbf{f} + \int_{\Omega} d_{\mathbf{u}} \mathbf{V}^T \boldsymbol{\lambda} \, d\Omega, \quad (6)$$

subject to the constraints

$$\nabla \cdot \mathbf{u} = 0, \quad \mathbf{V}(t_0 + \Delta t) \geq 0, \quad \boldsymbol{\lambda} \geq 0, \quad \boldsymbol{\lambda} \cdot \mathbf{V}(t_0 + \Delta t) = 0.$$

2.5. Complementary Problem

Given a configuration \mathbf{q}^n at t_n we can solve for the velocity without any repulsion \mathbf{u}^* by solving the system,

$$\mathbf{u}^* = \mathbf{A}(\mathbf{q}^n),$$

where $\mathbf{A}(\mathbf{q}^n)$ is some linear system arising from a discretization of the Stokes equations. To include the contributions to the velocity from the Stokes equations we can add an additional term,

$$\mathbf{u} = \mathbf{u}^* + \boldsymbol{\lambda} \mathbf{B} \mathbf{f}_c,$$

Where \mathbf{B} is some linear mapping from the repulsion force $\boldsymbol{\lambda} \mathbf{f}_c$ to an induced velocity. Once we have the velocity the configuration can be updated using an explicit Euler step,

$$\mathbf{q}^{n+1} = \mathbf{q}^n + \Delta t \mathbf{u}^n.$$

The complementary conditions can be stated as

$$\mathbf{V}(\mathbf{q}^n, \mathbf{u}) \geq 0 \perp \boldsymbol{\lambda} \geq 0.$$

Since \mathbf{u} depends on $\boldsymbol{\lambda}$, so does \mathbf{V} and in general this relationship is nonlinear. To linearize this constraint we can use a first order Taylor series expansion of \mathbf{V} to get

$$\mathbf{V}(\mathbf{q}^n, \mathbf{u}) = \mathbf{V}(\mathbf{q}^n, \mathbf{u}^* + \boldsymbol{\lambda} \mathbf{B} \mathbf{f}_c) \approx \mathbf{V}(\mathbf{q}^n, \mathbf{u}^*) + d_{\mathbf{u}} \mathbf{V}(\mathbf{q}^n, \mathbf{u}^*) \cdot \mathbf{B} \mathbf{f}_c \boldsymbol{\lambda}.$$

This gives us a linear complementary problem, which we can solve for $\boldsymbol{\lambda}$,

$$\mathbf{V}(\mathbf{q}^n, \mathbf{u}^*) + d_{\mathbf{u}} \mathbf{V}(\mathbf{q}^n, \mathbf{u}^*) \cdot \mathbf{B} \mathbf{f}_c \boldsymbol{\lambda} \geq 0 \perp \boldsymbol{\lambda} \geq 0.$$

2.6. Boundary Integral Equation Representation

As discussed in section 2.4, the governing equations for this problem are the incompressible Stokes equations. There are many ways to solve these equations, here we will use *boundary integral equations* (BIEs). For the Stokes BIEs have many advantages over other numerical methods such as finite element or finite volume methods. A discussion of the benefits of BIEs for this problem can be found in [3].

2.6.1. Unbounded Domains

In an unbounded domain there will be an imposed background flow \mathbf{u}_∞ . We will use BIEs to solve for a velocity perturbation \mathbf{u}_p due to the boundary conditions on particles and solid walls.

The solution to the Stokes equations (1) with a homogeneous forcing function at a point \mathbf{x} inside a domain Ω can be expressed as an integral around the boundary of the domain $\partial\Omega$,

$$\mathbf{u}_p(\mathbf{x}) = \mathcal{D}[\boldsymbol{\eta}](\mathbf{x}) = \frac{1}{\pi} \int_{\partial\Omega} \frac{\mathbf{r} \cdot \mathbf{n}}{\rho^2} \frac{\mathbf{r} \otimes \mathbf{r}}{\rho^2} \boldsymbol{\eta}(\mathbf{y}) \, ds(\mathbf{y}), \quad (7)$$

where $\boldsymbol{\eta}$ is an unknown density function defined only along $\partial\Omega$, $\mathbf{r} = \mathbf{x} - \mathbf{y}$ and $\rho = |\mathbf{r}|$. The operator $\mathcal{D}[\boldsymbol{\eta}]$ is the double layer potential and can be derived from the fundamental solution of (1) [4, 8]. The double layer potential by itself cannot represent all possible flow fields. In particular it cannot represent flows around surfaces undergoing a net force or torque. Following [6, 7] for surfaces undergoing an arbitrary net force \mathbf{F} and net torque L we can complete the double layer potential as,

$$\mathbf{u}(\mathbf{x}) = \mathbf{u}_\infty + \mathcal{D}[\boldsymbol{\eta}] + \sum_{i=1}^{N+M} (\mathbf{S}(\mathbf{x}, \mathbf{c}_i) \mathbf{F}_i + \mathbf{R}(\mathbf{x}, \mathbf{c}_i) L_i),$$

where the Stokeslet $\mathbf{S}(\mathbf{x}, \mathbf{y})$ and rotlet $\mathbf{R}(\mathbf{x}, \mathbf{y})$ are given by

$$\mathbf{S}(\mathbf{x}, \mathbf{y}) = \frac{\mathbf{r} \otimes \mathbf{r}}{\rho^2} - \log \rho \mathbf{I}, \quad \mathbf{R}(\mathbf{x}, \mathbf{y}) = \frac{\mathbf{r}^\perp}{\rho^2}.$$

Note that we have also added back in the background flow.

To set up a system to solve we can take the limit of (7) as we approach $\partial\Omega$ and match it to the boundary condition (2). The double layer potential is not continuous when we cross the boundary and has a limiting value of $-\boldsymbol{\eta}/2$. This leads to the second kind Fredholm equation,

$$-\frac{1}{2} \boldsymbol{\eta}(\mathbf{x}) + \mathcal{D}[\boldsymbol{\eta}](\mathbf{x}) + \sum_{i=1}^{N+M} (\mathbf{S}(\mathbf{x}, \mathbf{c}_i) \mathbf{F}_i + \mathbf{R}(\mathbf{x}, \mathbf{c}_i) L_i) = \mathbf{u}_b - \mathbf{u}_\infty. \quad (8)$$

On solid walls we will prescribe the velocity \mathbf{u}_b and solve for the net force and torque on each wall. This is called the *resistance problem*. For particles on the other hand we will prescribe the net force and torque on each particle and solve for the velocity \mathbf{u}_b . This is known as the *mobility problem*. We will use the fact that the particles are rigid to decompose \mathbf{u}_b into a translational and rotational component,

$$\mathbf{u}_b = \mathbf{u}^\tau + \omega(\mathbf{x} - \mathbf{c})^\perp.$$

This lets us set up an equation to solve for the velocity on the surface of particle k ,

$$-\frac{1}{2} \boldsymbol{\eta}(\mathbf{x}) + \mathcal{D}[\boldsymbol{\eta}](\mathbf{x}) - \mathbf{u}_k^\tau - \omega(\mathbf{x} - \mathbf{c}_k)^\perp = - \sum_{i=1}^{N+M} (\mathbf{S}(\mathbf{x}, \mathbf{c}_i) \mathbf{F}_i + \mathbf{R}(\mathbf{x}, \mathbf{c}_i) L_i) - \mathbf{u}_\infty. \quad (9)$$

For the both the resistance and mobility problem we have more unknowns than equations. In particular, we have to solve for two components of $\boldsymbol{\eta}$ and either

- (a) two components of net force and a net torque for each solid wall \rightarrow an additional $3M$ unknowns
- (b) two components of translational velocity and an angular velocity of each particle \rightarrow an additional $3N$ unknowns

To close these systems we will follow [6] and relate $\boldsymbol{\eta}$ to the net force and torque on each particle or wall. In particular for $1 \leq i \leq N + M$,

$$\int_{\Gamma_i} \boldsymbol{\eta} \, ds = \mathbf{F}_i, \quad (10a)$$

$$\int_{\Gamma_i} \boldsymbol{\eta} \cdot (\mathbf{x} - \mathbf{c})^\perp \, ds = L_i. \quad (10b)$$

Combining (8), (9) and (10) we can write our problem in the compact notation,

$$\begin{bmatrix} -\frac{1}{2} + \mathcal{D} & 1 & (\mathbf{x} - \mathbf{c})^\perp & \mathcal{S} & \mathcal{R} \\ \int \cdot ds & 0 & 0 & 0 & 0 \\ \int \cdot (\mathbf{x} - \mathbf{c})^\perp ds & 0 & 0 & 0 & 0 \\ \int \cdot ds & 0 & 0 & -1 & 0 \\ \int \cdot (\mathbf{x} - \mathbf{c})^\perp ds & 0 & 0 & 0 & -1 \end{bmatrix} \begin{bmatrix} \boldsymbol{\eta} \\ \mathbf{u}^\tau \\ \boldsymbol{\omega} \\ \mathbf{F}_w \\ \mathbf{L}_w \end{bmatrix} = \begin{bmatrix} -\mathbf{u}_\infty - \mathcal{S}\mathbf{F}_p - \mathcal{R}\mathbf{L}_p \\ \mathbf{F}_p \\ \mathbf{L}_p \\ 0 \\ 0 \end{bmatrix} \quad (11)$$

2.6.2. Bounded Domains

Bounded domains lead to a similar system, however it must be modified slightly. For fluid inside a container the double layer potential has a rank one null space [4]. Following [6] this null space can be removed by adding an operator that is active only over the enclosing boundary Γ_0 ,

$$\mathcal{N}_0[\boldsymbol{\eta}](\mathbf{x}) = \delta_{i0} \int_{\Gamma_i} \mathbf{n}(\mathbf{x}) \otimes \mathbf{n}(\mathbf{y}) ds(\mathbf{y}).$$

The compatibility condition (3) ensures that this term evaluates to 0. Adding \mathcal{N}_0 to (11) and removing the background flow leads to the linear system,

$$\begin{bmatrix} -\frac{1}{2} + \mathcal{D} + \mathcal{N}_0 & 1 & (\mathbf{x} - \mathbf{c})^\perp & \mathcal{S} & \mathcal{R} \\ \int \cdot ds & 0 & 0 & 0 & 0 \\ \int \cdot (\mathbf{x} - \mathbf{c})^\perp ds & 0 & 0 & 0 & 0 \\ \int \cdot ds & 0 & 0 & -1 & 0 \\ \int \cdot (\mathbf{x} - \mathbf{c})^\perp ds & 0 & 0 & 0 & -1 \end{bmatrix} \begin{bmatrix} \boldsymbol{\eta} \\ \mathbf{u}^\tau \\ \boldsymbol{\omega} \\ \mathbf{F}_w \\ \mathbf{L}_w \end{bmatrix} = \begin{bmatrix} -\mathcal{S}\mathbf{F}_p - \mathcal{R}\mathbf{L}_p \\ \mathbf{F}_p \\ \mathbf{L}_p \\ 0 \\ 0 \end{bmatrix} \quad (12)$$

2.7. Incorporating Repulsion Forces

The addition of a forcing term to the right hand side of the Stokes equations would normally lead to a volume integral. However, in this case since $d_{\mathbf{u}}V$ can be non-zero only on the boundary, we can capture the repulsion force by adding a net force and torque to each particle or wall as needed. The net force \mathbf{F}_p^k and torque L_p^k are given by,

$$\mathbf{F}_p^k = \int_{\Gamma_k} d_{\mathbf{u}}V^T \boldsymbol{\lambda} ds, \quad L_p^k = \int_{\Gamma_k} d_{\mathbf{u}}V^T \boldsymbol{\lambda} \cdot (\mathbf{x} - \mathbf{c}_k)^\perp ds.$$

3. Numerical Methods

The linear system (11) or (12) is discretized using a collocation trapezoid method. For particles that are in near-contact the near singular integration scheme described in [9, 11] is used. The discretized system is solved with GRMES [10] with a block diagonal preconditioner and accelerated using the fast multipole method [1]. Since the linear system arises from a second kind Fredholm equation the condition number of the matrix is bounded and does not increase with finer resolution. The number of GMRES iterations is therefore mesh resolution independent. This leads to a solver that is $O(n)$, where n is the number of mesh points.

Once we solve for the translational and angular velocity of the particles, the position and angle of each particle are updated according to the ODEs,

$$\frac{d}{dt} \mathbf{c}_k = \mathbf{u}_k^\tau, \quad \frac{d}{dt} \theta_k = \omega_k.$$

The ODEs are advanced in time using an explicit Euler step.

The matrices described in (11) and (12) are full. They can be made block-diagonal by treating inter-particle interactions explicitly and moving them to the right hand side. This is termed *locally implicit* and is described in [5]. For dense suspensions however this type of time stepping can lead to instabilities as particles become tightly packed.

4. Results

- One of the main results is that the new time integrator can handle higher concentrations
- Two bodies in extensional
- Multiple bodies in extensional and/or Taylor-Green
- Couette with low and high concentration

5. Conclusions

An appendix

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