A Fast Stokes Solver for Generalized Flow Problems

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ABSTRACT

Computing drag forces on geometrically complicated 3-D micromachined structures, such as an entire comb resonator, is a challenging problem. The recently developed FastStokes solver, based on precorrected-FFT accelerated iterative methods, has made analyzing such problems much less expensive. For this reason, there have been several extensions to the program to analyze unsteady flow and to improve computational efficiency. In this paper we develop several additional extensions to FastStokes. In particular, the direct BEM formulation is used to allow mixed velocity-pressure boundary conditions. We demonstrate the accuracy of the numerical approach by comparing computed results to the results from the indirect BEM formulation and low frequency asymptotic expansions for an oscillating sphere with Dirichlet boundary conditions. We show the ability of this solver to handle problems with mixed boundary conditions. Finally, the drag force on a micro-resonator packaged in the air is presented.

Keywords: Unsteady Stokes Flow, Boundary Element Methods, Precorrected FFT Techniques, Microfluidic Devices, Micro-resonator

INTRODUCTION

Analysis of the behavior of micromachined devices packaged in air or fluid requires the determination of drag forces and traction distribution on the devices due to the surrounding fluid. Since the spatial scales are small, the fluid can often be analyzed by neglecting the convective term. That is, one can assume the flow is governed by the Stokes equations. Even with this simplification, the geometrically complicated nature of most three-dimensional microfludic devices makes them expensive to simulate with standard finite- element or finite difference based Stokes flow solvers. The recently developed FastStokes solver[1], based on precorrected-FFT accelerated iterative methods[2], has made analyzing such problems much less expensive. For this reason, there have been several extensions to the program to analyze unsteady flow[3] and to improve computational efficiency[4].

In this paper we develop several additional extensions to FastStokes. In particular, the direct BEM formulation is used to allow mixed velocity- pressure boundary conditions, but the formulation requires extensions to the analytic integration formulas and the precorrected-FFT interface described in [3]. In the next section, we describe the boundary-element approach to solving the frequency-domain unsteady Stokes equations using the direct formulation and briefly describe the precorrected-FFT algorithm. In sections 3 and 4 we describe the extensions required by this formulation, that of computing integrals of the frequency-domain traction Green's functions and implement of this function in the precorrected-FFT algorithm. Next, we describe results using the developed program. We demonstrate the accuracy of the this approach by comparing computed results to our previous results based on the indirect BEM formulation[3] for an oscillating sphere. The drag force on a micro-resonator packaged in the air is also presented, to show that the method can be used to analyze practical problems. Finally, in Section 6, we give conclusions and acknowledgments.

FORMULATION

In the frequency domain, the direct boundary integral equations for unsteady Stokes flow are [5]

$$u_j(\mathbf{x_0}) = -\frac{1}{4\pi\mu}\int_S [f_i(\mathbf{x})G_{ij}(\hat{\mathbf{x}}) - \mu u_i(\mathbf{x})T_{ijk}(\hat{\mathbf{x}})n_k(\mathbf{x})]ds \tag{1}$$

where S is the surface on the object in an infinite fluid, and the two Greens' functions are given by [5]

$$G_{ij}(\hat{\mathbf{x}}) = \frac{\delta_{ij}}{r}A(R) + \frac{\hat{x}_i\hat{x}_j}{r^3}B(R); \tag{2}$$

$$T_{ijk}(\hat{\mathbf{x}}) = -\delta_{ik}2\frac{\hat{x}_j}{r^3} + \frac{\partial G_{ij}}{\partial x_k}(\hat{\mathbf{x}}) + \frac{\partial G_{kj}}{\partial x_i}(\hat{\mathbf{x}}). \tag{3}$$

$$A = 2e^{-R}(1+\frac{1}{R}+\frac{1}{R^2}) - \frac{2}{R^2} \tag{4}$$

$$B = -2e^{-R}(1+\frac{3}{R}+\frac{3}{R^2}) + \frac{6}{R^2} \tag{5}$$

$$R = \lambda r. \tag{6}$$

In (1), $u_j(\mathbf{x_0})$ is the jth component of the velocity vector at the source point $\mathbf{x_0}$, $\mathbf{f}$ is the Stokeslet density function that corresponds to the surface traction, $\mathbf{n}$ is the normal vector, ρ and μ are the density and the viscosity of the fluid respectively, $\hat{x_i}$ is the ith component of the relative position vector between the source point and the field point, i.e. $\hat{x_i} = x_{0i} - x_i$, r is the length of the relative position vector ($r = |\mathbf{x_0} - \mathbf{x}|$), λ is the frequency parameter which is defined as $\lambda^2 = i\omega\frac{\mu d^2}{\rho}$, ω is the frequency of the fluid and d is the characteristic size of the object.

If a piece-wise constant collocation scheme is used to solve (1)[6], then the surface of the object is discretized into n small panels and the unknown quantity, either the Stokeslet density function $\mathbf{f}$ or the velocity $\mathbf{u}$, is assumed to be uniformly distributed on each panel. A system of equations for the panel unknowns is then derived by insisting (1) is satisfied at each panel centroid. The result is a system which relates the known vector $\mathbf{b}$ to the unknown vector $\mathbf{x}$, as in

$$\begin{Bmatrix} \mathbf{b}^1 \\ \mathbf{b}^2 \\ . \\ . \\ . \\ \mathbf{b}^n \end{Bmatrix} = P(\omega) \begin{Bmatrix} \mathbf{x}^1 \\ \mathbf{x}^2 \\ . \\ . \\ . \\ \mathbf{x}^n \end{Bmatrix} \tag{7}$$

where $\mathbf{b}^i$ and $\mathbf{x}^i$ are the known and unknown vectors at the ith panel, P is a $3n \times 3n$ matrix whose elements are given by one of two cases. If $\mathbf{f^j}$ is unknown, then

$$P_{kl}^{ij}(\omega) = \int_{\Delta j} \left[\frac{\delta_{kl} A(R)}{|\mathbf{x}^i - \mathbf{x}|} + \frac{(x_k^i - x_k)(x_l^i - x_l)}{|\mathbf{x}^i - \mathbf{x}|^3} B(R) \right] ds \qquad k, l = 1, 2, 3. \tag{8}$$

Otherwise, if $\mathbf{u^j}$ is unknown,

$$P_{kl}^{ij}(\omega) = \int_{\Delta j} \left[-2\delta_{lm} \frac{x_k^i - x_k}{|\mathbf{x}^i - \mathbf{x}|^3} + \frac{\partial G_{lk}}{\partial x_m} + \frac{\partial G_{mk}}{\partial x_l} \right] n_m ds.$$

Above, $\mathbf{x}^i$ denotes the centroid of the ith panel and Δj denotes the surface of the jth panel.

SOLUTION ACCELERATION

The linear system in (7) can be solved to compute the unknown quantities. In this paper, instead of the direct approach, e.g. Gaussian Elimination, an iterative method, complex GMRES[7], is employed to solve the system. This reduces the computing time from $O(n^3)$ to $O(n^2)$. To further accelerate the computation, a precorrected FFT technique[2] is employed. This technique computes the matrix-vector product in $O(n \log n)$ operations. Thus, for problems with reasonably homogeneous distributions of panels, our code has $O(n \log n)$ complexity.

In the precorrected FFT approach, the problem domain is first divided into a three-dimensional array of small equal sized cubes, where the cube size is selected so that each cube contains a small number of panels (typically less than 20). The shared vertex points of the cubes form a uniform coarse grid, and this grid is used both to separate nearby panels (panels in adjacent cubes) from distant panels (panels in nonadjacent cubes). The interaction between nearby panels is computed directly in the standard fashion, and the interaction between distant panels is computed by projecting onto, and interpolating from, the coarse grid.

The implementation of the precorrected-FFT algorithm then consists the following four major steps (for the purpose of illustration, in the following paragraph, the unknown vectors are assumed to be the panel forces).
1. project the panel forces onto a uniform grid of point forces.
2. compute the grid velocities due to grid forces by performing a fast convolution using an FFT.
3. interpolate the grid velocities onto the panels.
4. directly compute nearby interactions.

The projection of panel forces onto the grid, and the interpolation of panel velocities from the grid, are performed using polynomial interpolation [5]. Each panel is projected onto a small number of surrounding grid points (typically 27), and each velocity is interpolated from a small number of surrounding grid points (also typically 27). It should be noted, however, that the Stokes flow problem is a vector problem, and therefore three force components must be projected and three velocities must be interpolated. Another Stokes flow specific issue is that the integral equation (2) includes two different Green's functions, and care must be taken to handle the various Green's functions efficiently. Finally, the nearby interactions require the evaluation of integrals with singular and near singular kernels. In the next two sections we discuss the nearby and grid interaction calculations.

NEARBY INTERACTION

In the direct BEM formulation, the calculation of the interaction of nearby panels needs the evaluations of the integrals of two unsteady Stokes Greens' functions, G and T, over the panels. In simplified form, the integrals to be evaluated are

$$I_1 = \int_{\Delta} [\frac{\delta_{ij}}{r} A(R) + \frac{\hat{x}_i \hat{x}_j}{r^3} B(R)] ds \tag{9}$$

$$I_2 = \int_{\Delta} [-2\delta_{ik} \frac{\hat{x}_j}{r^3} + \frac{\partial G_{ij}}{\partial x_k}(\hat{\mathbf{x}}) + \frac{\partial G_{kj}}{\partial x_i}(\hat{\mathbf{x}})] n_k ds \tag{10}$$

where r, $\hat{x}_i$, $\hat{x}_j$, A and B are as described above.

As shown in [3], I_1 can be evaluated accurately by exploiting the fact that the unsteady Stokes Greens function becomes the steady Stokes Greens' function as $\lambda \rightarrow$

0. To evaluate I_2, again we separate it into two parts. Let

$$I_2 = I_{21} + I_{22} \tag{11}$$

where

$$I_{21} = \int [-6\frac{\hat{x_i}\hat{x_j}\hat{x_k}}{r^5} n_k] ds \tag{12}$$

$$\begin{aligned} I_{22} &= \int \{-\frac{2}{r^3}(\delta_{ij}\hat{x_k} + \delta_{kj}\hat{x_i})[e^{-R}(R+1) - B] \\ &- \frac{2}{r^3}\delta_{ik}\hat{x_j}(1-B) \\ &- 2\frac{\hat{x_i}\hat{x_j}\hat{x_k}}{r^5}[5B - 2e^{-R}(R+1) - 3]\} n_k ds \end{aligned} \tag{13}$$

Note that I_{21} is the integral of the steady Stokes Greens' function. It is evaluated analytically using an extension of the techniques described in [3]. The integrand of the second integral, I_{22}, is a smooth function of r. This can be easily proved by examining the Taylor series expansion of the integrand about $R = 0$. Numerical quadrature is used to evaluate this part. In the near singular cases, i.e., when r is very close to 0, the Taylor series expansion of the integrand of I_{22} is used to compute the values of this integrand at Gaussian points to avoid the cancellation errors.

GRID INTERACTION

Using the direct BEM formulation in (2) has ramifications for the precorrected-FFT method. The term $\int_S [u_i(\mathbf{x}) T_{ijk}(\hat{\mathbf{x}}) n_k(\mathbf{x})] ds$ contains several Green's function components, and this can make computing the grid interactions expensive. To evaluate the needed quantities on the grid, one could project the nine panel quantities $u_i n_k$ onto the grid and then evaluate integrals with the 27 T_{ijk} components using 27 convolutions. There is a more efficient approach that can be derived by noting that the traction Greens' function T is a linear combination of the derivatives of the unsteady Stokeslet Greens' functions G and the potential Greens' function $\frac{1}{r}$, i.e.

$$T_{ijk} = 2\frac{\partial(\frac{1}{r})}{\partial x_k} + \frac{\partial G_{ij}}{\partial x_k} + \frac{\partial G_{kj}}{\partial x_i}. \tag{14}$$

The derivatives of the Greens' functions, for example, $\frac{\partial G_{ij}}{\partial x_k}$, can be represented approximately using weighted combinations of G_{ij} at m grid points as in

$$\frac{\partial G_{ij}}{\partial x_k} \approx \sum_m w_m G_{ij}^m \tag{15}$$

where the grid points are the ones which surround the panel, and m is equal to the number of points used in projection and interpolation (again typically 27).

Table 1: A sphere in an oscillating flow, Dirichlet boundary condition

	Direct BEM Formulation		Indirect BEM Formulation		Kanwal's solution	
ω	Drag.r	Drag.i	Drag.r	Drag.i	Drag.r	Drag.i
0.0	18.7947	0.0	18.8155	0.0	18.8496	0.0
0.0001	18.9273	0.1328	18.9441	0.1291	18.9828	0.1331
0.001	19.2141	0.4213	19.2354	0.4266	19.2710	0.4215
0.01	20.122	1.347	20.1429	1.395		
0.1	22.9926	4.408	22.9831	4.884		

Thus, instead of projecting $u_i n_k$ directly onto the grid, we project weighted $u_i n_k$'s onto the grid. This reduces the number of the convolutions from 27 to 7. This can be seen clearly in the following equation,

$$\begin{aligned} \int_S [u_i(\mathbf{x}) T_{ijk}(\hat{\mathbf{x}}) n_k(\mathbf{x})] ds &= 2\sum_m \frac{1}{r_m}(u_i n_i w_j^1)_m \\ &+ \sum_m G_{ij}^m (u_i n_k w_k^2)_m \\ &+ \sum_m G_{kj}^m (u_i n_k w_i^3)_m, \end{aligned} \tag{16}$$

where w^1, w^2, w^3 are the weighted functions associated with different Greens' functions.

RESULTS

Withour loss of generality, we assumed unit kinematic viscousity in the following numerical examples except the micro-resonator. First, a sphere oscillating in an unbounded viscous fluid with velocity $u = u_0 e^{i\omega t}$ was simulated. The drag forces exerted on the sphere at different frequencies obtained using the direct BEM formulation are shown in Table (1), together with the results calculated from the indirect BEM formulation and the asymptotic solutions (Kanwal's solutions [6]) at low frequencies. In these experiments, only Dirichlet boundary condition were considered. Results show a good agreement between the direct and indirect BEM formulations. The slightly lost accuracy in the direct formulation is due to the fact that the right-hand side vector of the linear system (7) is also calculated approximately using the precorrect-FFT technique. In the indirect formulation, the right-hand side vector is exact.

The major advantage of the direct BEM formulation is that it allows mixed velocity-pressure boundary conditions. Table (2) shows the drag force for the same sphere with velocity boundary conditions on half of the sphere and pressure boundary conditions on the other half. The analytic solutions were used to prescribe the boundary conditions in the steady case. The total number of panels used in the simulation was 3072.

One application of this solver is to accurately compute the drag force on a micro-resonator which leads to

Table 2: Drag force for the sphere moving uniformly in an infinite fluid flow, mixed boundary condition.

Direct BEM Formulation	Analytic Solution
18.7834	18.8496

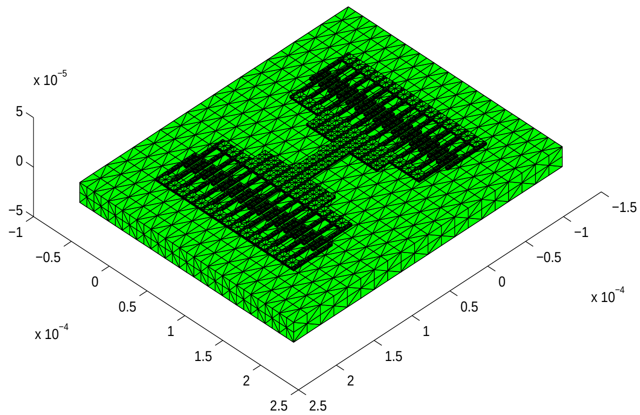

Figure 1: A micro-resonator with a substrate underneath

the predition of the quality factor of this device. The micro-resonator is oscillating in the air above a silicon substrate. Figure (1) shows the meshed micro-resonator and the substrate. Total drag force acting on the resonator is $171.33nN$. The time to compute the drag force using direct methods (for example, the Gaussian elimination) would have been 550 hours, but using the fast solver, the drag force can be computed in 32 minutes in the indirect BEM formulation and one hour in the direct BEM formulation.

CONCLUSIONS AND ACKNOWLEDGMENTS

In this paper we described the extensions made to FastStokes, a precorrected-FFT accelerated unsteady Stokes solver. In particular, the direct BEM formulation is used to allow mixed velocity-pressure boundary conditions. We demonstrated the accuracy of the numerical approach by comparing computed results to the results from the indirect BEM formulation and low frequency asymptotic expansions for an oscillating sphere with Dirichlet boundary conditions. We showed the ability of this solver to handle problems with mixed boundary conditions. Finally, the drag force on a micro-resonator packaged in the air was presented.

The authors would like to thank Narayan Aluru for his help with the FastStokes code and Joel Phillips for providing the precorrected-FFT code for use in this project. This work was supported by the DARPA composite CAD program.

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