# Fast Fluid Analysis for Multibody Micromachined Devices

X. Wang P. Mucha J. White
Department of Electrical Engineering and Computer Science, M.I.T. Cambridge, MA. 02139
email:white@mit.edu, FAX: (617) 258-5846, Phone: (617) 253-2543
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## Abstract

Recently developed fast integral equation methods for computing solutions to the Stokes' equation have proven to be a valuable tool for micromachined device designers. The speed of these fast codes make it possible to simulate multiple interacting 3-D structures, but issues associated with the singularity of the integral form of Stokes' equation have not been sufficiently carefully addressed to reliably perform such simulations. In this paper we describe the issue and show a remedy.

**Keywords:** Boundary Elements Methods, integral equation, singular operator, Stokes flow, micro-fluidic devices.

## Introduction

The recently developed precorrected-FFT accelerated boundary-element technique for fast solution of the Stokes equation has proved to be a valuable tool for micromachined device designers[1,2,3]. Codes based on these techniques are capable of determining the drag force on an entire comb structure in minutes, and the results have been used to demonstrate the inaccuracies of commonly accepted simplified analytic models[3]. The speed of these fast codes make it possible to simulate multiple interacting structures, but issues associated with the singularity of the integral form of Stokes' equation[4,5] have not been sufficiently carefully addressed to reliably perform such simulations.

The partial differential equations for Stokes' flow depends only on the gradient of pressure. This implies that any integral formulation for Stokes flow which directly relates forces to velocities can not have a unique solution, and therefore the linear system generated by discretizing the integral form will be precisely or nearly singular. If that singularity is not treated carefully, the resulting computed solution will be corrupted. Below we describe several techniques for dealing with the singularity of the discretized incompressible Stokes equation. In order to eliminate the null space in the linear system solution one can constrain the type of discretization and then properly apply a Krylov-subspace algorithm, but a more robust approach is to add a rank-one matrix to eliminate the discretized system's null space. Once the null-space free solution has been computed, a second step must be performed which introduces a pressure equation and pressure boundary condition to modify the null-space-free solution, so that the final solution of the Stokes equation is uniquely determined. Numerical examples are given to prove the effectiveness of our methods.

## Singular BEM Operators

The small feature size of micromachined devices implies that the fluid flow has a very low Reynolds number, and therefore the convective term in the Navier-Stokes equation can be neglected. The resulting simplification, the linear Stokes equation, can be solved using integral equations. In this paper we will only consider the steady incompressible Stokes equation, though the approaches described herein extend to the unsteady incompressible Stokes equation or even the linearized compressible Stokes equation. Assuming zero body force, the steady Stokes equation is

$$\begin{cases} -\nabla p + \mu \nabla^2 u = 0 \\ \nabla \bullet u = 0 \end{cases} \tag{1}$$

with stress tensor and surface force vector expressed as:

$$\sigma_{3\times 3} = -PI_{3\times 3} + \mu[\nabla u + (\nabla u)^T]$$

$$f_{3\times 1} = \sigma_{3\times 3} n_{3\times 1} \tag{2}$$

That only the derivative of pressure arises explicitly in the Stokes' equation implies that any constant pressure can be added to the solution of the Stokes' equation, and therefore the equation is singular. This constant-pressure zero-velocity solution is a "singular mode" which does not effect the total force on a single rigid body, but the singularity can impact the results produced by a numerical procedure. In addition, the detailed fluid forces on the body will not be computed correctly unless the singular mode is treated properly.

Fast solvers, such as the precorrected-FFT accelerated methods[2] are applied to integral forms of the Stokes' equation

$$u_i = -\frac{1}{8\pi\mu}\int G_{i,j} f_j ds$$

$$P = -\frac{1}{8\pi}\int p_i f_i ds \tag{3}$$

$$G_{i,j} = \frac{\delta_{i,j}}{r} + \frac{\hat{x}_i \hat{x}_j}{r^3}, \qquad p_i = 2\frac{\hat{x}_i}{r^3}$$

We assume the fluid motion is generated by the motions of rigid bodies, so the single layer potential is used in the above equations. The integral operator whose kernel is $G$ is a singular operator whose nullspace is the outward normal to the body surface. That is,

$$\int_{surface} G_{i,j}\vec{n} ds = 0 \tag{4}$$

A common approach to discretizing (3) is to use a collocation scheme in which the unknowns are a discrete set of surface traction forces, denoted by the vector $F$, and the knowns are a discrete set of collocation point velocities, denoted by $U$. If the above integral formulation is used to compute fluid forces on a problem with $m$ moving bodies, a collocation scheme will generate a system of equations $U = GF$, where $G$ is now the discrete form of the integral operator with an m-dimension nullspace given by the outward-normal vectors of the m objects in the system. The fact that G has an m-dimensional nullspace implies that the surface force can not be uniquely determined from $U = GF$ system of equations alone. If net body forces, and not detailed surface forces, are all that are of interest, then the nullspace components can simply be eliminated in the computation procedure. Otherwise, it is necessary to remove the unwanted null space part and make sure the solution is unique and correct.

## Approaches

If a Krylov-subspace based method, such as GMRES, is used to solve $U = GF$, the procedure will converge to a null-space free solution under certain conditions. In particular, the $G$ matrix must be symmetric, so an exact Galerkin-style discretization would be needed, and the the right-hand side must be perpendicular to the nullspace. If the right-hand side is not perpendicular to the nullspace or the discretization scheme generates only a nearly symmetric $G$ matrix, then the Krylov-subspace method may fail. A more numerically robust approach to computing a null-space free solution is to use rank-one matrices to augment the G matrix. For an m-object system, if $F$ is any solution satisfying $GF = U$ and $F^{\perp}$ is the null-space free solution, then $G'F^{\perp} = U$ where

$$G' = G + \sum_{i=1}^{m} c_i N_i N_i^T, \tag{5}$$

$N_i$ is the normal vector of the $ith$ object, $c_i$ is a constant such chosen that the values of the rank-one matrix elements are moderately small comparing with those in the $G$ matrix. Since the $G'$ matrix is no longer singular, the equation can be easily be solved and

$$(G + \sum_{i=1}^{m} c_i N_i N_i^T)F^{\perp} = GF^{\perp} = GF = U. \tag{6}$$

The above methods give a unique solution that is perpendicular to the nullspace of the G matrix, but the actual solution may contain nullspace components. For example, consider the two plate problem in Figure 1 below, in which a top plate approaches a bottom plate. Assume that the nullspace component of the force is zero, in this case the nullspace is the plate surface normal. Then, the normal force on the side of the moving plate facing the fixed plate must be equal in magnitude and opposite in sign to the force on the side of the plate facing away from the fixed plate, and this is clearly non-physical. If detailed plate surface forces are desired, pressure must be taken into consideration.

From the original Stokes equation, it is clear that a pressure boundary condition is necessary to compute a unique solution, either a $P_\infty$ or a $P_{certain-point}$. Assume $P_\infty$ is given, then the pressure is given by

$$P = -\frac{1}{8\pi}\int p_i f_i ds + P_\infty \tag{7}$$

Even though the surface force solution of $U = GF$ is not unique due to the nullspace of $G$ matrix, the solution of pressure $P$ is unique for any solution $F$ because $p_i$ has a corresponding singularity. Note the normal direction force is $f_n = n^T_{1\times 3}\sigma_{3\times 3}n_{3\times 1}$ We use the following relation to modify the surface forces solution:

$$F_n^{point} = -P^{point} + 2\mu\frac{\partial u_n^{point}}{\partial n} = -P^{point} \tag{8}$$

Here $F_n^{point}$ is the normal direction surface force of a point on the surface. $\frac{\partial u_n}{\partial n} = 0$ since non-slip boundary assumption is applied. If $F'$ is the solution $F^\perp$ of the first two methods mentioned above or any solution satisfying $GF' = U$, and let $C = -P - F_n^\perp$, then

$$F_{final} = F^\perp + C^{point} \cdot N_i \tag{9}$$

is the solution which satisfies both the Stokes equation and the pressure boundary condition. Only one $P^{point}$ is needed to calculate the $C^{point}$ for each surface. Theoretically, $C$ should be the same at any point on the surface, but discretization error and other numerical error may affect the accurate of $C$. A straight forward conclusion is that $C$ at points far from corners and boundary are more accurate.

## Results

Results from applying the above methods to a two-plate problem are shown in Figures 1 and 2 below. In the two-plate example, the top plate is moving at velocity $V_z = 1$ while the bottom plate is fixed. The size of the two plates are $100\mu m \times 100\mu m \times 15\mu m$. Figure 1 shows the result of ignoring the singularity, and the second picture shows the result of using the pressure pinning method above. Although not obvious from the figures, the first method gives the correct total forces, but it is quite clear that only the second one gives the correct surface force distribution.

The FastStokes simulation results from a comb drive structure is shown in Figure 3 and 4. The comb shuttle is moving at velocity $V_x = 1$, the side combs and the substrate are fixed. Figure 4 shows a reasonable detailed force distribution.

## Conclusions

In this paper we noted that the singularity of the incompressible Stokes equation has not been sufficiently carefully addressed. By introducing a pressure integral equation and using an appropriate numerical algorithm, the unique and correct solution of the system can be achieved without substantial additional effort. Finally, detailed surface force plots demonstrate the effectiveness of the method described.

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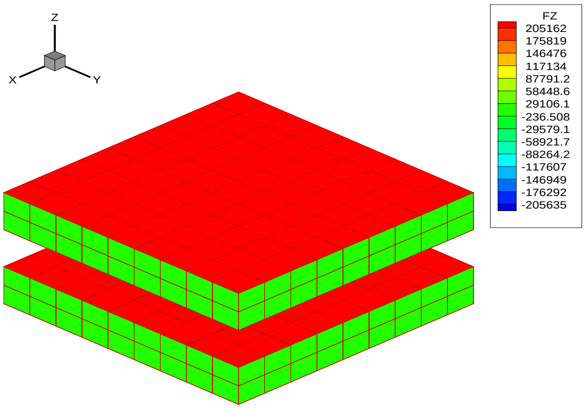


Figure 1: Wrong surface forces

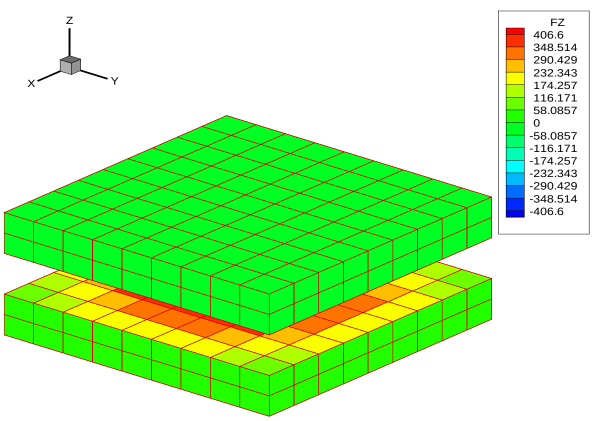


Figure 2: Surface forces using pressure-pinning

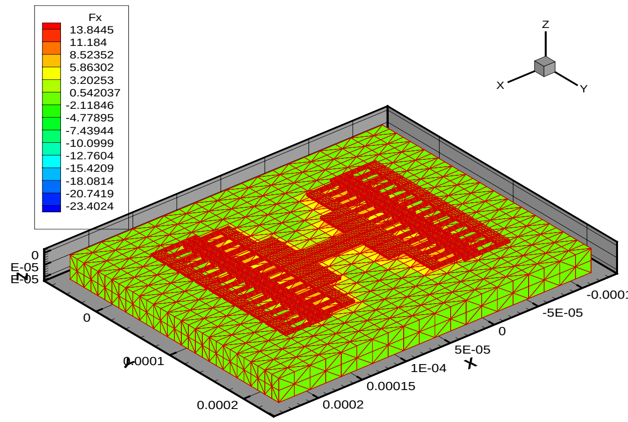


Figure 3: Surface force distribution on a comb-drive structure

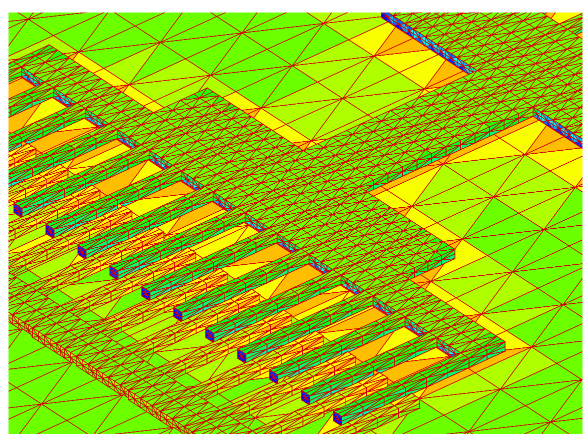

Figure 4: Surface forces on different objects