Fast Multipole accelerated BE techniques for 3D Stokes flow

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Summary

A procedure for the evaluation of drag forces due to Stokes flow around complex Micro-Electro-Mechanical-Systems (MEMS) is discussed. The proposed technique makes use of discretized boundary integral equations. Both single-layer and double-layer formulations are analysed. Numerical tests are carried out on three selected geometries.

Introduction

MEMS, though being a promising and revolutionary technology, still suffer several design difficulties due to their intrinsic complexity. One of the open issues in MEMS design is the simulation of the fluid flow around moving parts. Due to the small scale of MEMS, which implies low Reynolds numbers even for fast oscillating parts, turbolence can be safely neglected, and the resulting Stokes model can be employed to evaluate the viscous drag actions exerted on moving parts.

Boundary integral equation methods appear to be a viable approach for the effective solution of viscous incompressible flow on external domains ([6],[7]). The use of the Fast Multipole Method [4] for the evaluation of matrix-vector multiplications allows to solve, with a reasonable computational cost, the large-scale problems required by complex boundary geometries.

The resistance problem

With reference to a 3D situation, one or more rigid bodies of surface Γ_α are moving with assigned velocity in a viscous, incompressible fluid, which can be either unbounded or confined in an enveloping rigid boundary Γ_E. The total drag force and torque acting on these bodies are sought.

The steady-state Stokes flow is governed by

$$\begin{cases} \mu \Delta \boldsymbol{u} - \nabla P = 0 \\ \nabla \cdot \boldsymbol{u} = 0 \end{cases} \tag{1}$$

where $\boldsymbol{u}$ is the flow velocity, P is the hydrodynamic pressure and μ is the viscous drag coefficient.

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In the resistence problem a rigid motion velocity at each surface Γ_α is assigned

$$\boldsymbol{u}|_{\Gamma_\alpha} = \boldsymbol{V}_\alpha + \boldsymbol{\Omega}_\alpha \times \boldsymbol{X} \tag{2}$$

A free flow must also satisfy the radiation condition at infinity

$$\lim_{x\to\infty} \boldsymbol{u}(x) \; = \; O\left(|x|^{-1}\right) \tag{3}$$

while confined flows must match the velocity of the enclosing boundary

$$\boldsymbol{u}|_{\Gamma_E} = \boldsymbol{V}_E + \boldsymbol{\Omega}_E \times \boldsymbol{X} \tag{4}$$

The single-layer formulation

Assuming an external flow around multiple rigid bodies, the velocity at any point of the domain can be expressed in terms of a single-layer hydrodynamic potential $\boldsymbol{q}$, leading to the equation

$$u_i(x_0) \; = \; -\int_\Gamma u_i^j(x,x_0)\, q_j(x)\, \mathrm{d}S(x) \tag{5}$$

where

$$u_i^j(x,x_0) \; = \; \frac{1}{8\pi\mu}\, \frac{\delta_{ij}}{r} + \frac{(x-x_0)_i\,(x-x_0)_j}{r^3} \qquad r \; = \; |x-x_0| \tag{6}$$

is called *stokeslet*. This equation holds even at points belonging to the boundary, due to the weakly singular nature of the kernel. The unknown potential $\boldsymbol{q}$ is the surface traction exerted by the fluid flow over the rigid surfaces Γ_α.

It can be shown [6] that (5) is a singular operator. In order to solve the resistance problem it is necessary to impose the orthogonality of the solution to the null-space of the homogeneous operator associated to (5). Since the basis of the null-space is described by the normal vectors to the surfaces of the rigid bodies, the additional set of constraints has the form

$$\int_{\Gamma_\alpha} q_j(x)\, n_j(x)\, \mathrm{d}S_\alpha \; = \; 0 \qquad \forall\alpha \tag{7}$$

thus imposing a null hydrostatic pressure over each surface Γ_α. The use of these constraints allows to find a solution $\boldsymbol{q}_\perp$. The correct solution differs from $\boldsymbol{q}_\perp$ by a set of constant hydrostatic pressures p_α applied to each surface. These pressures can be evaluated by means of a pressure integral equation; however they are ignored here since they do not contribute to total force and total torque. The latter quantities can be evaluated by direct integration of the tractions over each surface Γ_α.

The theory of first kind Fredholm integral equations shows that (5) can lead to ill-conditioned problems. However, an assessment of the actual limitations of this approach when applied to large-size problems still deserves further study ([2], [3]).

The completed double-layer formulation

According to an alternative approach, the velocity at any internal point of the flow region can be expressed as a function of a double-layer density $\boldsymbol{\phi}$, through the equation

$$u_i(x_0) = -\int_\Gamma K_{ij}(x, x_0)\,\phi_j(x)\,\mathrm{d}S(x) \tag{8}$$

where

$$K_{ij}(x, x_0) = \frac{3}{4\pi\mu}\frac{(x-x_0)_i\,(x-x_0)_j\,(x-x_0)_k\,n_k(x)}{r^5} \qquad r = |x - x_0| \tag{9}$$

is called *stresslet*.

When the point x_0 is taken to the boundary from the external domain, the strongly singular nature of the stresslet kernel gives rise to a free term. The resulting boundary integral equation at a smooth boundary point is

$$u_i(x_0) = \frac{1}{2}\phi_i - \int_\Gamma K_{ij}(x, x_0)\,\phi_j(x)\,\mathrm{d}S(x) \qquad x \in \Gamma \tag{10}$$

where the integral exists in the Cauchy Principal Value sense. Equation (8) cannot describe an arbitrary solution of (1) since it can be shown that (10) has a solution only if the assigned velocity condition over each boundary surface satisfies the constraint

$$\begin{gathered}\int_{\Gamma_\alpha} u_j(x)\,\psi_j^{k,(\alpha)}(x)\,\mathrm{d}S = 0 \\ \psi_j^{k,(\alpha)} = \delta_{jk} \qquad \psi_j^{k+3,(\alpha)} = \varepsilon_{jkl}\,(x - x_\alpha)_l \qquad k = 1,2,3\end{gathered} \tag{11}$$

where x_α is an arbitrary point internal to surface Γ_α. The rigid body velocity assigned to the boundary surfaces does not satisfy (11), thus it leads to a velocity field that cannot be described in terms of a double-layer potential alone. Moreover, the generic flow described by (8) decays at infinity with order $O(1/r^2)$, contradicting the radiation condition for unbounded flows.

Power and Miranda ([5]) proposed a *completed formulation*, which describes the velocity field in the form

$$\begin{aligned} u_i(x_0) = &-\int_\Gamma K_{ij}(x, x_0)\,\phi_j(x)\,\mathrm{d}S(x) + \\ &\sum_\alpha u_i^j(x_0, x_\alpha)\,F_j^{(\alpha)} + \sum_\alpha r_i^j(x_0, x_\alpha)\,M_j^{(\alpha)} \end{aligned} \tag{12}$$

where

$$r_i^j(x_0, x_\alpha) = \frac{1}{8\pi\mu} \frac{\varepsilon_{ijk}(x_0 - x_\alpha)_k}{r^5} \tag{13}$$

is called *rotlet*.

The stregth of the internal singulatities can be arbitrarily expressed as linearly dependent upon the double-layer density:

$$\begin{aligned} F_k^{(\alpha)} &= \int_{\Gamma_\alpha} \phi_j(x)\, \psi_j^{k,(\alpha)}(x)\, \mathrm{d}S \\ M_k^{(\alpha)} &= \int_{\Gamma_\alpha} \phi_j(x)\, \psi_j^{k+3,(\alpha)}(x)\, \mathrm{d}S \end{aligned} \tag{14}$$

The completed double-layer equation can be solved in terms of the unknown double-layer density. Due to the properties of stresslet, stokeslet and rotlet, the total force acting on the generic body α is equal to $F^{(\alpha)}$; analogously, the total torque with respect to the point x_α is equal to $M^{(\alpha)}$.

Implementation

The discretization of both (5) and (12) by means of the collocational Boundary Element Method is a quite straightforward task. In order to allow the solution of large problems, the GMRES iterative solver coupled with the Fast Multipole Method ([4], [1]) has been implemented. Various approximations, from piecewise constant to piecewise linear, have been tested. The orthogonality constraints required by the single-layer formulation have been satisfied by imposing them on each search direction of the iterative solver.

Numerical examples

As a first test, the drag force exerted on a sphere and on a cube subject to a pure translation in an unbounded domain is evaluated. Five different formulations are tested: single-layer with piecewise constant approximation (SLPC), and double-layer with piecewise constant (DLPC), continuous linear (DLCL), piecewise linear (DLPL) and partially piecewise linear (DLPPL) approximation. DLPPL formulation is discontinuous only across edges of the cubic geometry.

Figure 1 shows the error in the evaluation of the drag force using different meshes and formulations. The reference value is represented by the analytical one in the case of the spherical body, and by the value obtained with a 150000 DOF mesh using the single-layer formulation for the cubic body.

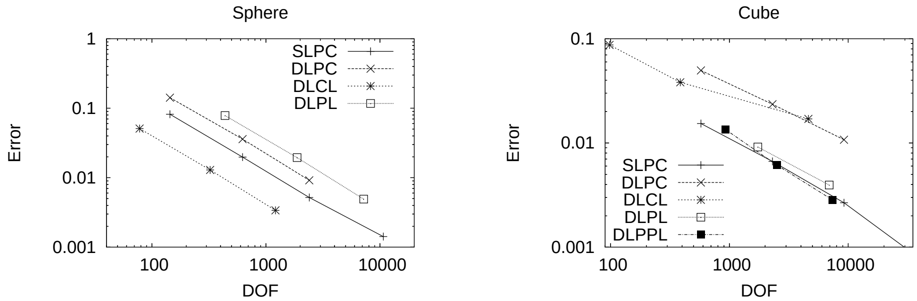

Figure 1: Error on the total drag force evaluation on a translating sphere and cube

The second example which is discussed is a first attempt to solve a complex geometry resembling an actual MEMS. The comb-drive resonator shown in Figure 2 is made of thee parts: two fixed stators and a rotor which is allowed to translate parallel to the finger axis direction. The main dimension of the model is 215 μm, and the air viscosity coefficient is set to $\mu = 1.73 \times 10^{-5}\ N\ s\ m^{-2}$.

The total drag force acting on the rotor is evaluated using the single-layer formulation and three different meshes. The following table shows the results obtained, together with the time needed to solve the problems on a Pentium 4 3GHz PC.

DOF	F (nN)	Matrix-vector multiplication time (s)	Iterations	Total time (s)
28800	138.24	8	29	284
145572	144.69	102	32	3777
368220	147.78	275	34	11661

Conclusions

This contribution presents some preliminary results of a research work that is still under way. Several issues are being addressed, mainly related to ill-conditioning in the presence of complex geometries. The goal of this work is to create a BE tool for applied research in MEMS design and prototyping.

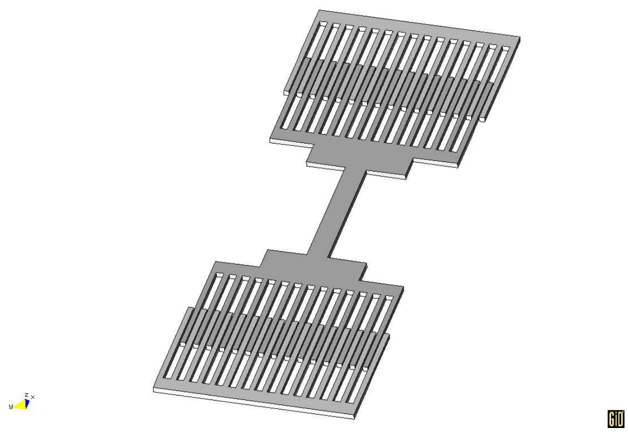

Figure 2: Comb-drive resonator geometry

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