Dealing with stiffness in time-domain Stokes flow simulation

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Abstract

As microfluidic devices become more common and more elaborate, it becomes necessary to develop simulation tools that allow the efficient and yet accurate three-dimensional time-domain analysis of the behavior of these devices. Detailed time domain analysis of three dimensional microfluidic structures requires dealing with the stiffness of the differential equations associated with the motion of objects in viscous fluids and with updating the solver grids. We minimize the issue of mesh adaptation by using the boundary element method which only requires discretizing and updating two dimensional surface meshes. We address the issue of stiffness by introducing a velocity implicit time stepping scheme that has much better stability than the explicit Forward Euler scheme and that has a much lower computational cost than a fully implicit scheme.

1 Introduction

In microfluidics we are usually dealing with very small scales and relatively slow velocities. In these conditions, the Reynolds number is very low and the fluid motion is dominated by viscous terms. These devices are operating in the Stokes flow regime[1].

In microfluidic devices developed for biological and medical applications it is often the case where there are cells or other objects moving in the fluid[2]. Manipulating cells and other objects in microfluidic systems requires the understanding of how the control forces and the fluid forces acting on the objects interact[3]. Time domain analysis of the behavior of the controlled objects and their interaction with, often complicated geometries, is very useful to optimize the actuators, the control system and microfluidic chamber design [4]–[6].

The time-domain equations associated with the motion of bodies in a very viscous fluid are very stiff. In order to capture the overall movement of the body and maintain stability using an explicit time integrating scheme, very small time-steps must be used. Even with fast solvers, this limitation on the time step seriously limits the behaviors that can be simulated. Stiffness is usually dealt with by using an implicit time integration method. In this case, a fully implicit method would require solving a set of non-linear equations involving the dependency of the fluid force on the position and the velocity of the objects. However, even though the fluid forces are non-linearly dependent on the position of the objects, they depend linearly on the object velocities. It turns out that, because the fluid is very viscous at these length scales, the fluid force on a body traveling inside the fluid is very strongly dependent on the velocity of the body and not as much on incremental changes on its position. We have dealt with the stiffness issue by introducing a *velocity-implicit* time integration scheme. By identifying that the stiffness of the equations came from the dependency of the fluid force on an object on its velocity and not as much on its position, we could safely just solve a linear system at each time-step and were able to eliminate the need to solve the non-linear space-dependent equation.

To calculate the force acting on the moving objects at each time step we use a boundary element method[7]. The boundary element method is particularly suitable for use with time integration as it only requires the discretization of the surfaces of the domain. Furthermore, at each time step, only the mesh of the objects that are moving need to be updated. This approach contrasts with volume discretization methods where the fluid domain is also meshed and must be updated at each time step[8].

This paper is structured as follows. In section 2, we review Stokes flow. In section 3, we present a boundary element formulation using pressure and velocity boundary conditions. In section 4 we discuss the issue of time integration and introduce the velocity implicit time stepping method. In section 5 we present some results obtained with the velocity implicit technique. Finally in section 6, we discuss the advantages and limitations of our approach.

2 Background information

If the Reynolds number $Re = UL/\nu$ is small, the viscous term in the Navier-Stokes equations dominates over the convective term and we get the Stokes equations

$$\rho\frac{\delta \mathbf{u}}{\delta t} = -\nabla p + \mu\nabla^2\mathbf{u} + \mathbf{b}. \quad (1)$$

where $\mathbf{u}$ is the velocity field, p is the pressure and $\mathbf{b}$ are body forces applied to the fluid. We assume that the fluid is imcompressible i.e. that $\nabla \cdot \mathbf{u} = 0$. Note that incompressibility is not a necessary condition for Stokes flow. Also note that, while the Navier-Stokes equations are non-linear in $\mathbf{u}$, due to the convective term, the Stokes equations are linear.

We further simplify (1) by assuming that we are operating in a quasi-static regime. In these conditions the time derivative term vanishes and we get

$$\begin{cases} -\nabla p + \mu \nabla^2 \mathbf{u} + \mathbf{b} = 0 \\ \nabla \cdot \mathbf{u} = 0 \end{cases} \tag{2}$$

If a point force $\mathbf{g}$ is applied at $\mathbf{x}_0$ i.e. if $\mathbf{b}(x) = \delta(x - x_0)\mathbf{g}$, the value of the velocity, pressure and stress tensor are given by

$$\begin{array}{rcl} u_i(\mathbf{x}) & = & \frac{1}{8\pi\mu} G_{ij}(\hat{\mathbf{x}}) g_j = \frac{1}{8\pi\mu}\left(\frac{\delta_{ij}}{r} + \frac{\hat{x}_i \hat{x}_j}{r^3}\right) g_j \\ P(\mathbf{x}) & = & \frac{1}{8\pi} p_j(\hat{\mathbf{x}}) g_j = \frac{1}{4\pi}\frac{\hat{x}_i}{r^3} g_j \\ \sigma_{ik}(\mathbf{x}) & = & \frac{1}{8\pi} T_{ijk}(\hat{\mathbf{x}}) g_j = -\frac{3}{4\pi}\frac{\hat{x}_i \hat{x}_j \hat{x}_k}{r^5} g_j \end{array} \tag{3}$$

where $\hat{\mathbf{x}} = \mathbf{x} - \mathbf{x}_0$ and $r = \|\hat{\mathbf{x}}\|_2$, and σ_{kj} is the fluid stress tensor

$$\sigma_{kj} = -P\delta_{ij} + \mu\left(\frac{\delta u_i}{\delta x_k} + \frac{\delta u_k}{\delta x_i}\right) \tag{4}$$

where P is the pressure (for the derivation see [7]).

2.1 Lorentz reciprocity

An integral equation formulation of a pressure driven fluid flow problem can be constructed by using the Lorentz reciprocity theorem [7]. The Lorentz reciprocity theorem states that, given two solutions A and B of two problems with different boundary conditions but in the same fluid domain, the velocities and stress tensors are related by

$$\frac{\delta}{\delta x_j}\left(u_k^A \sigma_{kj}^B - u_k^B \sigma_{kj}^A\right) = u_k^A \frac{\delta \sigma_{kj}^B}{\delta x_j} - u_k^B \frac{\delta \sigma_{kj}^A}{\delta x_j} = 0. \tag{5}$$

This equality holds if there are *no externally applied forces* at the point of evaluation. The Lorentz reciprocity condition is very useful for defining boundary conditions.

If we integrate (5) over a fluid domain V excluding objects and points were external forces are applied (and (5) does not hold) and use the divergence theorem we get

$$\int_V \frac{\delta}{\delta x_j}\left(u_k^A \sigma_{kj}^B - u_k^B \sigma_{kj}^A\right) dV = \int_V u_k^A \underbrace{\sigma_{kj}^B \mathbf{n}_j}_{f_k^B} dV - \int_V u_k^B \underbrace{\sigma_{kj}^A \mathbf{n}_j}_{f_k^A} dV = 0 \tag{6}$$

where f_k^B represents the force applied to the fluid along the kth direction and where $\mathbf{n}$ is the exterior normal surface vector (pointing away from the fluid).

If solution A is associated with an external unit force applied at point $\mathbf{x}_0$ and pointing along the ith axis, we get $u_k^A = G_{k,i}$ and $\sigma_{kj}^A = T_{k,i,j}$. This yields a set of three equations of the form

$$\int_{\delta V} \frac{1}{8\pi\mu} G_{ki}(\mathbf{x}-\mathbf{x}_0) f_k^B(\mathbf{x}) dA - \int_{\delta V} u_k^B(\mathbf{x}) \frac{1}{8\pi} T_{kij}(\mathbf{x}-\mathbf{x}_0)\mathbf{n}_j dA = 0. \tag{7}$$

Note that the point $\mathbf{x}_0$ must be excluded from the integration domain for (5) to hold. To do this we decompose V as $\hat{V} - S_\epsilon(\mathbf{x}_0)$ where $S_\epsilon(\mathbf{x}_0)$ represents an infinitesimal sphere of radius ϵ centered on $\mathbf{x}_0$. As ϵ goes to zero the equation becomes

$$\int_{\delta\hat{V}} G_{ki}(\mathbf{x}-\mathbf{x}_0) f_k^B(\mathbf{x}) dA - \mu \int_{\delta\hat{V}} u_k^B(\mathbf{x}) T_{kij}(\mathbf{x}-\mathbf{x}_0)\mathbf{n}_j dA = 8\pi\mu u_i(\mathbf{x}_0). \tag{8}$$

3 Boundary Element Method

In pressure driven microfluidic systems, we are usually dealing with pressure boundary conditions at the device's inlets and outlets and with no-slip, no penetration velocity boundary conditions at the device walls. We are then faced with determining the forces applied to the moving objects in the system and updating the position and velocity of these moving objects.

In this paper, we consider a fluid domain that is bounded by a set of surfaces. These surfaces are the device walls, open fluid surfaces at the inlets and outlets and the surfaces of the objects moving inside the device.

Since (8) is bilinear in the velocity and force at $\mathbf{x}_0$, if we only use and evaluation point per panel we must know either the velocity or the force applied at each point or we must have a relationship between these values such that the number of unknowns is the same as the number of constraints.

For now we assume that the either we know the fluid velocity or the forces applied to the fluid at each point. We discretize the surface $\delta\hat{V}$ into a finite set of triangular or quadrangular flat panels. We approximate the value of the velocity and the force applied to the fluid at each panel by a constant value. Let $\mathbf{U}$ and $\mathbf{F}$, in $\mathbb{R}^{n_{panels}\times 3}$, represent the fluid velocity and forces applied to the fluid just outside each panel.

$$\sum_{n=1}^{n_{panels}} F_{n,k} \int_{P_n} G_{ki}(\mathbf{x}-\mathbf{x}_0) dA - \mu \sum_{n=1}^{n_{panels}} U_{n,k} \int_{P_n} T_{kij}(\mathbf{x}-\mathbf{x}_0)\mathbf{n}_j dA = 8\pi\mu u_i(\mathbf{x}_0). \tag{9}$$

A system of linear equations can be formed by using collocation by setting $\mathbf{x}_0$ in (9) to be each of the panel centroids. We can then represent (9) in matrix form as

$$\mathbf{GF} - \mu(\mathbf{T} + 8\pi\mathbf{I})\mathbf{U} = 0 \tag{10}$$

where $\mathbf{F}$ and $\mathbf{U}$ are now vectors with $3n_{panel}$ entries.

If we assume we know either the velocity of the force on each surface we can split $\mathbf{F}$ into an unknown $\mathbf{F}_1$ and a known $\mathbf{F}_2$ and $\mathbf{U}$ into a known $\mathbf{U}_1$ and an unknown $\mathbf{U}_2$. By splitting $\mathbf{G}$ and $\mathbf{T}$ accordingly we have

$$\begin{bmatrix} \mathbf{G}_{11} & -\mu\mathbf{T}_{12} \\ \mathbf{G}_{21} & -\mu(\mathbf{T}_{22}+8\pi\mathbf{I}) \end{bmatrix} \begin{bmatrix} \mathbf{F}_1 \\ \mathbf{U}_2 \end{bmatrix} = \begin{bmatrix} \mu(\mathbf{T}_{11}+8\pi\mathbf{I}) & -\mathbf{G}_{12} \\ \mu\mathbf{T}_{21} & -\mathbf{G}_{22} \end{bmatrix} \begin{bmatrix} \mathbf{U}_1 \\ \mathbf{F}_2 \end{bmatrix} \tag{11}$$

which can then be solved for $\mathbf{F}_1$ and $\mathbf{U}_2$. Note that $\mathbf{F}_1$ are the fluid forces, right outside of the object boundary. By Cauchy's theorem, the forces applied to the body are the negative of the fluid forces.

For rigid objects whose surface are entirely in the surface integration domain

$$\int_{\delta Object} u_k(\mathbf{x}) T_{kij}(\mathbf{x}-\mathbf{x}_0)\mathbf{n}_j dA = 0. \tag{12}$$

We can use this result to avoid having to calculate the panel T integrals for the panels that form closed rigid objects.

4 Time stepping

In this section we start by establishing the connection between the boundary element bilinear form (11), an the acceleration and angular acceleration of mobile objects. We then review the forward Euler integration scheme and then present the velocity implicit time integration method.

In order to implement a time-stepping scheme we must, at some point, calculate the force distribution on the surface of each mobile object. This can be accomplished by using (11).

Assuming that during each time step the forces are constant, the object acceleration $\mathbf{a}$ and angular acceleration $\dot{\mathbf{w}}$ due to the surface stress forces are given by

$$\begin{array}{c} \mathbf{v}_{k+1} = \mathbf{v}_k + \Delta t \mathbf{a}_{k+1} = \mathbf{v}_k - \Delta t \mathbf{M}^{-1} \int_{\text{surface}} \mathbf{F}^{(q)}_{k+1} dS_q \\ \mathbf{w}_{k+1} = \mathbf{w}_k + \Delta t \dot{\mathbf{w}} = \mathbf{w}_k - \Delta t \mathbf{I}^{-1} \int_{\text{surface}} r^{(q)} \times \mathbf{F}^{(q)}_{k+1} dS_q \end{array} \tag{13}$$

Let p represent a point at the surface of the mobile object above and let $\mathbf{r}^{(p)}$ represent the vector from the object's center of mass to p, the velocity of p is given by

$$\mathbf{u}^{(p)}_{k+1} = \mathbf{v}_{k+1} + \mathbf{w}_{k+1} \times r^{(p)} = \underbrace{\mathbf{v}_k + \mathbf{w}_k \times r^{(p)}}_{=u^{(p)}_k} + \left(\mathbf{a}_k + \mathbf{w}_k \times r^{(p)}\right) \times r^{(p)}. \tag{14}$$

4.1 Forward Euler

As a first step, we implemented a fixed step Forward Euler integration scheme. The scheme can be summarized by the following equations

$$\begin{array}{rcl} \mathbf{F}_k & = & \mathbf{F}(\mathbf{x}_k, \theta_k, \mathbf{v}_k, \mathbf{w}_k) \\ \mathbf{M}\mathbf{a}_k & = & \mathbf{F}_k \\ \mathbf{v}_{k+1} & = & \mathbf{v}_k + \mathbf{a}_k \Delta t \\ \mathbf{x}_{k+1} & = & \mathbf{x}_k + (\mathbf{v}_k + 1/2\mathbf{a}_k \Delta t)\,\Delta t \\ \mathbf{I}\dot{\mathbf{w}}_k & = & \mathbf{r} \times \mathbf{F}_k \\ \mathbf{w}_{k+1} & = & \mathbf{w}_k + \dot{\mathbf{w}}_k \Delta t \\ \theta_{k+1} & = & \theta_k + (\mathbf{w}_k + 1/2\dot{\mathbf{w}}_k \Delta t)\,\Delta t \end{array} \tag{15}$$

where the k subscript indicates the time-step index.

The forward-Euler algorithm described above is too inefficient to be practical, because the method is stable only for very small values of Δt. The reason the forward Euler integrator is unstable and can only be used with very small time-steps is that the time-domain equations associated with the motion of bodies in a very viscous fluid are very stiff. In order to capture the overall movement of the body and maintain stability using an explicit time integrating scheme, very small time-steps must be used. Even with fast solvers, this limitation on the time step would seriously hinder the range of behaviors that can be simulated.

Usually, to deal with the stiffness issue, one would use an implicit time-integration scheme like backward-euler or the trapezoidal method. However, implementing an implicit integration scheme in $\mathbf{x}_{k+1}$ θ_{k+1}, $\mathbf{v}_{k+1}$ and $\mathbf{w}_{k+1}$ would require solving a geometric non-linear equation at each time step. The geometric non-linearity is associated with $\mathbf{x}_{k+1}$ and θ_{k+1}. Solving a nonlinear equation involving $\mathbf{x}_{k+1}$ and θ_{k+1} would require additional expensive evaluations of the kernel integrals in (11).

4.2 Velocity implicit scheme

The velocity implicit scheme is an intermediate, and much simpler approach, that takes advantage of the fact that the stiffness comes from the dependence of the force on velocity and not incremental changes of the position of mobile objects. The velocity implicit scheme also takes advantage of the fact that (13) and (14) both depend linearly on the panel forces $\mathbf{F}$. In this case, rather than using $\mathbf{v}_k$ and $\mathbf{w}_k$, which map to $\mathbf{U}_{1,k}$ in (11), to solve for $\mathbf{F}_k$ we can use $\mathbf{v}_{k+1}$ and $\mathbf{w}_{k+1}$ that map to $\mathbf{U}_{1,k+1} = \mathbf{U}_{1,k} + \Delta t \Delta U \mathbf{F}_{1,k}$. Going back to (11) in our formulation we get,

$$\begin{bmatrix} \mathbf{G}_{11} - \mu(\mathbf{T}_{11}+8\pi\mathbf{I})\Delta t \Delta\mathbf{U}(.) & -\mu\mathbf{T}_{12} \\ \mathbf{G}_{21} - \mu\mathbf{T}_{21}\Delta t \Delta\mathbf{U}(.) & -\mu(\mathbf{T}_{22}+8\pi\mathbf{I}) \end{bmatrix} \begin{bmatrix} \mathbf{F}_{1,k+1} \\ \mathbf{U}_{2,k+1} \end{bmatrix} = \begin{bmatrix} \mu(\mathbf{T}_{11}+8\pi\mathbf{I}) & -\mathbf{G}_{12} \\ \mu\mathbf{T}_{21} & -\mathbf{G}_{22} \end{bmatrix} \begin{bmatrix} \mathbf{U}_{1,k} \\ \mathbf{F}_{2,k+1} \end{bmatrix} \tag{16}$$

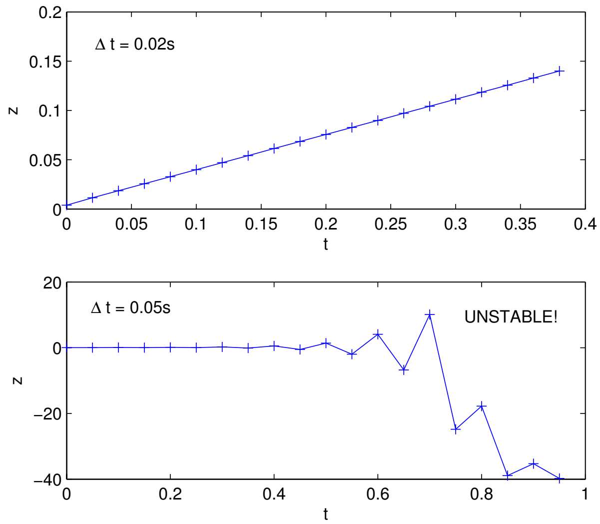
There is no need to represent $\Delta\mathbf{U}(.)$ explicitly because the linear system is solved using GMRES that only requires matrix vector products and therefore only requires applying the operator.

The velocity implicit scheme is much more stable than the forward Euler explicit scheme and is significantly less expensive and complicated than a fully implicit scheme.

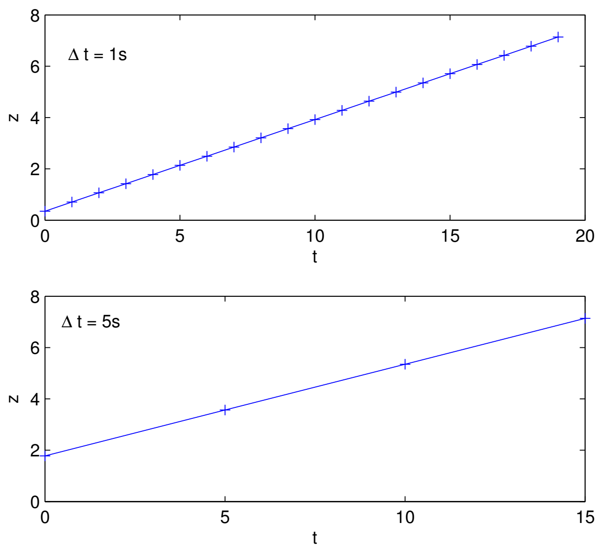
5 Results

An example of a sphere moving through a channel is illustrated in Figure 1. This example compares the velocity implicit method and the forward euler method.

For the same problem, the forward euler method becomes unstable for time steps above $0.04s$. The velocity implicit method allows steps of 5s and even higher.



a) Using explicit method must keep $\Delta t < 0.05$.



b) The velocity implicit scheme can take large time steps.

Figure 1: Velocity-implicit vs. explicit time domain integration scheme.

6 Conclusions

In this paper we have presented a velocity implicit time stepping scheme for the analysis of objects moving in Stokes flow. The velocity implicit scheme is motivated by the fact that the stiffness in the time integration of the fluid forces acting on the moving objects is associated with the velocity of the objects rather than their position. Using the velocity implicit scheme, rather than a fully implicit scheme on both velocity and position, avoids having to solve a non-linear equation at each time step and provides the stability that is absent in fully explicit schemes.

We have used a boundary element formulation of the Stokes flow problem to determine the forces applied at the surface of the moving objects. Boundary element methods are well suited for simulations with moving boundaries because of the reduced amount of mesh updating at each time step when compared to volume discretization methods.

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REFERENCES

[1] Xin Wang. *FastStokes: A Fast 3-D Fluid Simulation Program for Micro-Electro-Mechanical Systems.* PhD thesis, MIT, June 2002.

[2] J. Voldman, M.L. Gray, and M.A Schmidt. Microfabrication in biology and medicine. *Annu. Rev. Biomed. Engr.*, (1):401–425, 1999.

[3] J. Voldman. *A Microfabricated dielectrophoretic trapping array for cell-based biological assays.* PhD thesis, MIT, 2001.

[4] W. Ye and S. Mukherjee. Optimal three-dimensional analysis and design of electrostatic comb drives using boundary element method. *International Journal for Numerical Methods in Engineering*, (45):175–194, 1999.

[5] W. Ye, S. Mukherjee, and N. C. MacDonald. Optimal shape design of an electrostatic comb drive in micro-electromechanical systems. *Journal of Micro electromechanical Systems*, 7(1):16–27, 1998.

[6] P-C Yen and Y-J Yang. Time-domain reduced-order models of lateral viscous damping effects for 3-d geometries. In *Technical Proceedings of the 2002 International Conference on Modeling and Simulation of Microsystems*, volume 1, pages 190–193, 2002.

[7] C. Pozrikidis. *Boundary integral and singularity methods for linearized viscous flow.* Cambridge texts in applied mathematics. Cambridge University Press, 1992.

[8] David C Kring. *Time domain ship motions by a three-dimensional Rankine panel method author.* PhD thesis, MIT, 1994.