

FAST METHODS FOR PARTICLE DYNAMICS IN DIELECTROPHORETIC BIOCHIPS

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ABSTRACT

This paper introduces a Schur-complement based boundary element method (BEM) for predicting the motion of arbitrarily shaped three-dimensional particles under combined external and fluidic force fields. The BEM approach presented here relies entirely on modeling the surface of the computational domain, significantly reducing the number of unknowns when compared to volume-based methods. In addition, the Schur complement based scheme leads to a huge reduction in solution time during time-stepping in the microfluidic domain. Parallelized oct-tree based $O(N)$ multilevel iterative solvers are used to accelerate the setup and solution costs.

Keywords: BEM, cell-handling devices, microfluidics

1 INTRODUCTION

Many lab-on-chip (LoC) devices use dielectrophoretic (DEP) manipulation of polarized species inside microfluidic channels [1-3]. Understanding the fluidic and electromagnetic forces in these devices require rigorous treatment of the underlying physics. BEM based system matrix is dense in nature due to the highly coupled interaction between the wall and the particles, especially when the particle size is comparable to that of the channels (Fig. 1). Conventionally, the numerical treatment of such systems is achieved via brute-force computation of the whole fluidic domain during each time-step of the iteration. Hence, during computation of the motion of rigid or deformable particles a large number of time steps are required, where each time step consists of a computationally expensive solution of a dense matrix system. Previous work on Lab-on-chip modeling has been mainly based on finite-element and volume based methods [3-6,9]. The problem with these methods lie in the fact that they need to remesh the whole channel for each time step, while in BEMs only the surface is meshed, which significantly reduces the number of unknowns [6, 17, 18]. Here a scheme based on Schur-complement is presented to accelerate the time-stepping algorithm by partially decoupling wall-particle interactions. Particle motion can be predicted for arbitrarily shaped three-dimensional particles under combined external and fluidic force fields. Parallelized oct-tree based $O(N)$ multilevel iterative solvers

are used to accelerate the setup and solution costs [12-16]. In the past BEM techniques have been used to study low Re flows [8, 17], however, fast algorithms for dynamic systems remain a topic of active research [10]. Besides the fluidic fields, DEP fields are produced by on-chip electrodes. A coupled circuit-EM formulation is used for accurate prediction of DEP field distribution that allows circuit control of resulting electromagnetic fields [11] (fig 5). Simulations of particle trajectory in pressure-driven dielectrophoretic LoCs are presented. Evidence of applications of the current methodology to a large class of flow devices [7] for particle transport is presented.

2 INTEGRAL EQUATIONS

The integral representation for incompressible Stokes flow are given by the following expressions [17,18]:

$$u_i(\mathbf{x}_0) = \frac{-1}{4\pi\mu} \int_D G_{ij}(\mathbf{x}, \mathbf{x}_0) f_j(\mathbf{x}) dS(\mathbf{x}) + \frac{1}{4\pi} \int_D^{pV} u_j(\mathbf{x}) T_{ijk}(\mathbf{x}, \mathbf{x}_0) n_k(\mathbf{x}) dS(\mathbf{x})$$

No-slip and pressure boundary conditions are applied on the surface of the channel, while force and torque balance equations are setup for rigid particles,

$$\oint \boldsymbol{\sigma} \cdot d\mathbf{S} = \mathbf{F}_{ext}$$

$$\oint \mathbf{r} \times (\boldsymbol{\sigma} \cdot d\mathbf{S}) = \mathbf{T}_{ext}; \quad \mathbf{u}_{particle} = \mathbf{U} + \boldsymbol{\Omega} \times \mathbf{r}$$

\mathbf{U} and $\boldsymbol{\Omega}$ are the translation and angular velocities. The external forces and torques can be DEP fields for example. The surface of the domain is discretized using triangular patches and subsequently a collocation method is used for solving the unknown traction and velocity fields. The particle velocities can be solved at each time step and the resulting trajectory can be encountered for. However solving the whole dense matrix system for each time step becomes prohibitively expensive and an algorithm to reduce this cost is described below.

The first step in this algorithm is the isolation of the particle under study and is achieved by identifying the patches belonging to the mathematical surface bounding the particle \mathbf{S}_p . This surface isolates the problem into two parts – a subset of the problem which is constant over time

and another part which is changing over time. All the force and velocity unknowns belonging to the channel constitutes the first part (**D**) which consists of the single and double layer interactions of the channel walls and faces, whereas all the force unknowns belonging to the particle are represented by **A** which consists of the single layer interactions among the particle patches. Notice that this decomposition does not change integral equations of the equivalent problem with a change in the shape or location of the object bounded by \mathbf{S}_p . A small change in the shape of \mathbf{S}_p may not require additional patches, however if the shape and size of the particle changes drastically more patches have to be added to the particle surface to maintain a desired level of accuracy. As a result of decomposing the actual problem can be thought of as four different parts – the channel interacting with itself (**D**), the particle interacting with itself (**A**), the channel to particle interaction (**B**) and the particle to channel interaction (**C**). **B** contains both single and double layer interactions while **C** consists of single layer interactions only. The resulting system can be described by the following systems of equations:

$$\mathbf{D}\mathbf{y} + \mathbf{C}\mathbf{x} = \mathbf{a}_1$$

$$\mathbf{B}\mathbf{y} + \mathbf{A}\mathbf{x} = \mathbf{a}_2$$

Since the channel walls are static and unchanging in time the matrix **D** is constructed and stored in the form of its inverse - only once during the first time step. This is followed by updating the Schur's complement of the unchanging part (**D**) which is given by $\mathbf{S} = \mathbf{A} - \mathbf{B}\mathbf{D}^{-1}\mathbf{C}$, at each time step. The unknowns are then computed by back-substitution using a standard Schur complement method. Therefore for each step of the iteration the dimension of the net system is greatly reduced which saves considerable computational cost. It is important to note that the proposed technique bypasses the cost of explicit modeling of the mutual coupling between the channel walls and the particles.

Here the surface traction forces in both the channel and the particle problems are implemented and a simple case where the particle is treated as a rigid body and its shape is constant in time. However the methodology presented here is generally valid for deformable particles whose shape and size change over time. The surface of the channel supports both velocity and force unknowns while the particle surface supports only force unknowns. In order to take into account the translation and rotational velocities of the particle the net external force and torque have to be imposed on its surface. On the channel walls the three components of the velocities are set to zero in order to enforce no-slip conditions, whereas the traction forces on the channel faces are provided by the imposed pressure gradient. Note that the velocities on the channel faces are unidirectional. An appropriate preconditioner can be applied during use of a fast solver when required. The traction forces on particle surface are unknowns and the double layer contribution due to a closed particle is zero outside its boundary. Combining

all the interactions, along with the force and torque balance equations, the overall system is written in a matrix form:

$$\begin{bmatrix} \mathbf{D} & \mathbf{C} \\ \mathbf{B} & \mathbf{A} \end{bmatrix} \begin{bmatrix} \mathbf{f}_c \\ \mathbf{u}_c \\ \mathbf{f}_p \end{bmatrix} = \begin{bmatrix} \mathbf{p}_1 \\ \mathbf{p}_2 \\ \mathbf{F}_{ext} \\ \mathbf{T}_{ext} \end{bmatrix}$$

where \mathbf{f}_c are unknown traction forces on the channel surface, \mathbf{u}_c are the velocity unknowns at the faces and \mathbf{f}_p are the traction forces on particle surface. The known vector (RHS) represents the single layer contributions due to the imposed pressure at each face and excites the fluid flow. The other parts are sparse since they represent the summation of the surface forces on the particle and don't involve the channel patches. Typically for large complicated channels the number of unknowns on the channel surface greatly exceeds the particle surface. This implies the tacit assumption that the number of patches on particle \ll number of patches on the channel for the Schur complement based scheme proposed here to be an efficient solver. Fig. 2 shows the speedup due to the proposed scheme. It can be seen that for small number of particles the speedup factor is 5-6 times for each time step.

2.1 Algorithmic Complexity

If N_1, N_2, N_3 are the number of unknowns on the surfaces S_c, S_f and S_p , the cost of solving during the stages of the iterations where the appropriate blocks are pre-computed is given by C_1 , where

$$C_1 = N_1^3 + N_1 N_2 (N_1 + N) + N_1^2 + N_1 N_2 + N_2 N_3$$

If changing the excitation on the neighboring geometry is not required the cost can be further reduced to C'_1 given by

$$C'_1 = N_1^3 + N_1 N_2 (N_1 + N) + N_1^2 + N_1 N_2$$

The cost reduction is therefore given by a factor of N_3^3 / N_i^3 .

The expensive step in the iterations however is the computation of the Schur complement, i.e., during computing $\mathbf{D}^{-1}\mathbf{C}$. But as long as the number of particle patches is small, large speedups during time stepping can be achieved. Simulation examples are depicted in figs 1-5.

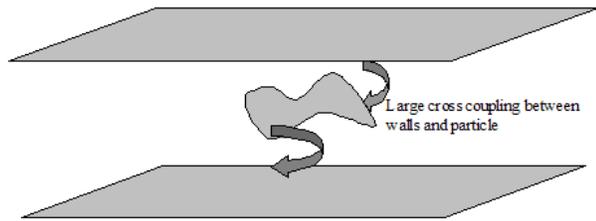


Fig 1: Cross-coupling due to interaction between channel wall and particle

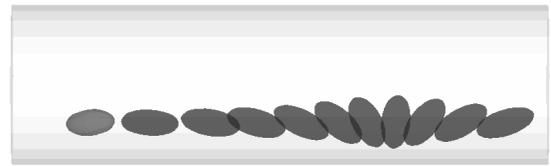


Fig 4: Simulation of platelet motion in a pressure driven micro-channel

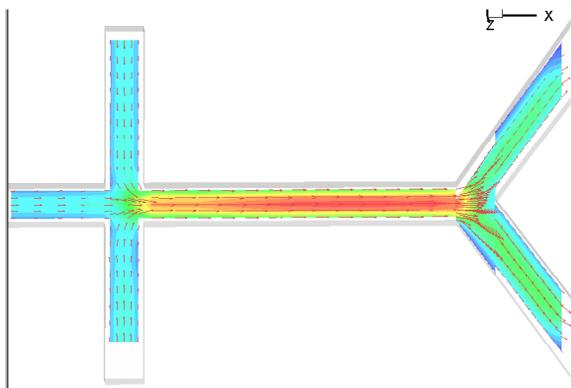


Fig 2: Flow field distribution in a complicated channel topology

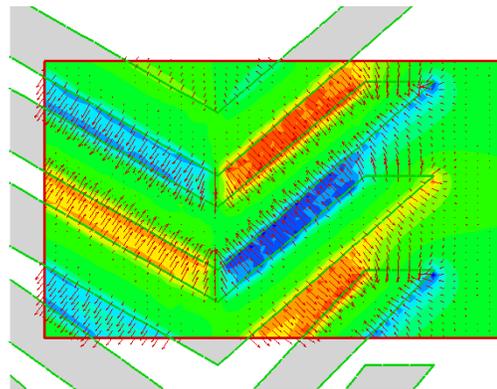


Fig 5 : DEP field distribution due to a V-shaped electrode array

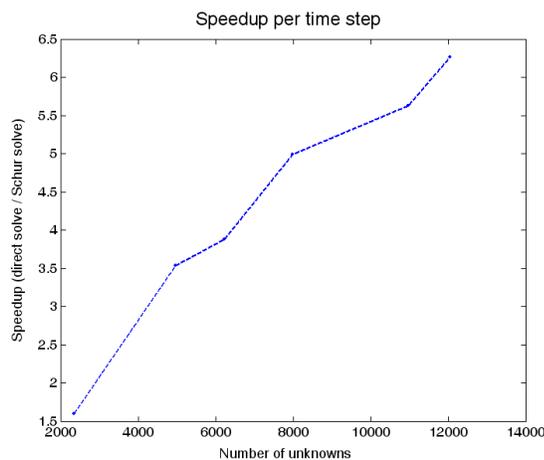


Fig 3: Speedup of solution time for solver

REFERENCES

- [1] Weigl BH, Bardell RL, Cabrera CR, *Lab-on-a-chip for drug development*, Adv Drug Deliv Rev. 2003, 3, pp. 349-77.
- [2] Gascoyne P. R., Vykoukal, *DEP based Sample Handling in General Purpose Programmable Diagnostic Instruments*, Proc IEEE, vol 92, no. 1(2004).
- [3] Haibo, L., Z. Yanan, A. Demir, and R. Bashir, *Characterization and Modeling of Microfluidic Dielectrophoresis Filter for Biological Species*, Journal of MEMS, Vol. 14 No. 1 (2005).
- [4] Wang, X, Wang X-B, Becker F. and Gascoyne P. R. C., *A theoretical method of electrical field analysis for dielectrophoretic electrode arrays using Green's theorem*, J. Phys. D: Appl. Phys., 29; pp. 1649-1660 (1996).
- [5] Clague, D.S., Wheeler EK, *Dielectrophoretic manipulation of macromolecules: The electric field*, Physical Review E, 64 (2): Art. No. 026605 Part 2, AUG 2001.

- [6] David Ericksson, *Towards numerical prototyping of labs-on-chip: modeling for integrated microfluidic devices*, *Microfluid Nanofluid* (2005), 1, pp. 301–318.
- [7] Barry Lutz, *Microeddies as Microfluidic Elements:Reactors and Cell Traps*, PhD thesis, University of Washington, 2003.
- [8] C. Pozrikidis, *Numerical Simulation of Cell Motion in Tube Flow*, *Annals of Biomedical Engineering*, 33, No. 2, February 2005, pp. 165–178.
- [9] R. Chein and S. H. Tsai, *Microfluidic Flow Switching Using Volume of Fluid Model*, *Biomedical Microdevices* 6: I, pp. 81-90, 2004.
- [10] Dong Liu, Martin Maxey, and George Karniadakis, *A Fast Method for Particulate Micrflows*, *Journal of MEMS*, 11, no. 6, 2002, pp. 691-702.
- [11] Y. Wang, D. Gope, V. Jandhyala and C.J. Shi, *Generalized KVL-KCL Formulation for Coupled Electromagnetic-Circuit Simulation with Surface Integral Equations*, *IEEE Transactions on. Microwave Theory Tech.*, vol. 52, no. 7, pp. 1673-1682, July 2004.
- [12] X. Wang, *FastStokes: A fast 3D fluid simulation program for MEMS*, PhD thesis, MIT (2002)
- [13] Senturia S. D, Aluru N., White J., *Simulation the behavior of MEMS devices: computational methods and needs*, *Comput. Sci. and Engg.*, IEEE, 4 (1997).
- [14] Gope D., Chakroborty S., Jandhyala V., *A Fast Parasitic Extractor Based on Low Rank Multilevel Matrix Compression for Conductor and Dielectric Modeling in Microelectronics and MEMS*, DAC 2004, 794-799.
- [15] Nabors K. and White J., *FastCap: A Multipole-Accelerated 3-D Capacitance Extraction Program*, *IEEE Transactions on Computer-Aided Design*, vol. 10, November 1991, p1447-1459.
- [16] I. Chowdhury and V. Jandhyala, *Single multilevel expansions and operators for potentials of the form $r^{-\lambda}$* , *SIAM J. Sci. Comput.*, vol. 26(2005), pp. 930-943.
- [17] Youngren G. K., Arcivos A., *Stokes flow past a particle of arbitrary shape: a numerical method of solution*, *J. Fluid Mech.*, 69 (1975).
- [18] C. Pozrikidis, *BI and singularity methods for linearized viscous flow*, Cambridge, 1992.