A Precorrected-FFT Method for Coupled Electrostatic-Stokes Flow Problem

Ngoc Son NGUYEN[1], **Kian-Meng LIM**[1], **Jacob WHITE**[2]

[1] *Singapore-MIT Alliance, E4-04-10, 4 Engineering Drive 3, Singapore 117576*
[2] *Singapore-MIT Alliance, Room 8-407, 77 Massachusetts Avenue, Cambridge, MA 02139 USA*

Abstract **- We present the application of the boundary integral equation method for solving the motion of biological cell or particle under Stokes flow in the presence of electrostatic field. The huge dense matrix-vector product from the boundary integral method poses a computationally challenging problem for solving the large system of equations generated. In our work, we used the precorrected-FFT (pFFT) method to reduce the computational time and memory usage drastically, so that large scale simulations can be performed quickly on a personal computer. Results on the force field acting on the particle, as well as the behavior of the particle through cell trap are presented.**

Keywords **– Boundary Element Method, Fast Fourier Transform, precorrected FFT, Electrostatic, Stokes flow.**

1. Introduction

We consider the problem of tracking particle motion in a micro-fluidic dielectrophoretic (DEP) cell-trap. The forces acting on the particle include the DEP and hydrodynamic forces, and the boundary integral equation (BIE) method is used to solve both the electrostatic and linearized viscous flow problems. However, this approach generates a dense matrix-vector system which is expensive to solve.

Several fast algorithms had been developed to improve the computational efficiency of BIE, such as the fast multipole method (FMM), hierarchical singular value decomposition (SVD), panel clustering method, and the pre-corrected FFT (pFFT). In this paper, we use the pFFT approach for accelerating the dense matrix vector product.

2. Problem Formulation

In the present work, two problems are solved: electrostatic problem and linearized viscous flow (or Stokes flow) problem.

2.1. Electrostatic problem

We consider the 3D problem of a sphere (with dielectric permittivity ε_p) in a cell-trap, with fluid medium of dielectric permittivity ε_f. The governing equation is the Laplace equation:

$$\nabla^2 \phi = 0$$

The integral equation is given by

$$c\phi(x_0) + \int_S \frac{dG(x_0,x)}{dn}\phi(x)dS(x) - \int_S G(x_0,x)\frac{d\phi(x)}{dn}dS(x) = 0 \qquad (1)$$

where c is 1 at an internal point, ½ for a point on 'smooth boundary' or 0 for a point outside the region Ω. The quantities ϕ and $d\phi/dn$ are the electrical potential and flux, respectively, and G is the 3D Laplace Green function:

$$G(x_0,x) = \frac{1}{4\pi\|x - x_0\|}.$$

We solve the integral equation (1) with the following boundary conditions:

1. Potential ϕ is given on the trap surfaces (S_2).
2. Flux $d\phi/dn$ on particle surface (S_1) satisfies:

$$\varepsilon_p \frac{d\phi^-}{dn} - \varepsilon_f \frac{d\phi^+}{dn} = 0$$

Combining the integral equations for both the domains inside and outside of the particle, we have:

$$\phi^{(1)}(x_0) + \int_{S_1} \frac{dG(x_0,x)}{dn}\phi^{(1)}(x)dS(x) - \int_{S_1} \frac{\varepsilon_f}{\varepsilon_p} G(x_0,x)\frac{d\phi^{(1)}(x)}{dn}dS(x) = 0$$

$$\phi(x_0) + \int_{S_1+S_2} \frac{dG(x_0,x)}{dn}\phi(x)dS(x) - \int_{S_1+S_2} G(x_0,x)\frac{d\phi(x)}{dn}dS(x) = 0$$

$$\phi^{(2)}(x_0) = V_0$$

A standard BEM approach using piece-wise constant collocation scheme is applied. The boundary surfaces are discretized into N panels, and we assume that ϕ and $d\phi/dn$ are uniformly distributed on each panel. This results in a dense linear system:

$$A\bar{x} = b \qquad \left(\bar{x} = \begin{bmatrix} \phi \\ d\phi/dn \end{bmatrix}\right)$$

The amplitude of the electric field is given by

$$\bar{E}_n = -\nabla\phi_n = -\frac{d\phi}{dn}\bar{n}$$

And the corresponding DEP force acting on the particle, arising from the non-uniform electric field and differences in dielectric properties is given by

$$\left\langle \overline{F}_{DEP} \right\rangle = \int_S (T.\overline{n}) dS$$

where *T* is the Maxwell stress tensor (MST):

$$T = \varepsilon_f \left(\overline{E}\overline{E}^* - \frac{1}{2}\left|\overline{E}\right|^2 I \right)$$

Here, ε_f is the permittivity of the fluid medium, and $\overline{E}^*$ is the complex conjugate of $\overline{E}$.

The Clausius-Mossotti (C-M) factor

$$K = \frac{\varepsilon_p - \varepsilon_f}{\varepsilon_p + 2\varepsilon_f}$$

determines whether the DEP force is positive (acts in the direction of increasing potential with *Re(K)>0*), or negative (acts in the direction of decreasing potential with *Re(K)<0*).

2.2. Stokes flow problem

Newtonian fluid flow at small values of the frequency parameter ($\beta = L^2 / \nu T$) and Reynolds number ($\mathrm{Re} = UL/\nu$) is governed by the Stokes equation

$$-\nabla P + \mu \nabla^2 u = 0$$

in addition to the continuity equation

$$\nabla . u = 0$$

The integral equation formulation gives

$$u_i(x_0) = \int_S G_{ij}(x_0, x) q_j(x) dS(x)$$

where q is the surface traction, and *G* is the 3D Stokes's Green function

$$G_{ij}(x_0, x) = \frac{\delta_{ij}}{r} + \frac{\overline{x}_i \overline{x}_j}{r^3}$$

where $\overline{x} = x - x_0$, $r = \left\|\overline{x}\right\|$.

The pressure and the stress fields are given by the corresponding distributions:

$$P(x_0) = \mu \int_S p_j(x_0, x) q_j dS(x)$$

$$\sigma_{ik}(x_0) = \mu \int_S T_{ijk}(x_0, x) q_j dS(x)$$

where p and T are the pressure vector and stress tensor, respectively, associated with the Green's function.

The force F exerted on the particle is given by

$$F = -8\pi\mu \int_S q dS$$

For this problem, we also use the piece-wise constant collocation scheme to solve for the integral equation, which results in a dense linear system

$$Aq = \overline{u}$$

where $\overline{u}$ is the vector of velocities.

2.3. Solving dense linear system

The discretized integral equation results a dense linear system of size $n \times n$, which is computationally expensive to solve.

Using Gaussian elimination to solve to solve the system will incur $O(n^3)$ operations. To improve the solution efficiency, we use an iterative method such as GMRES:

GMRES algorithm*:* $Ax = b$
Make an initial guess x^0
Set k = 0
do {
  Compute the residual: $r^k = b - Ax^k$
  if $\| r^k \| < tol$ *, return* q^k *as the solution*
  else {
    Find α*'s and* β *in:*

$$q^{k+1} = \sum_{j=0}^{k} \alpha_j q^j + \beta r^k$$

    to minimize $\| r^{k+1} \|$
    Set $k = k + 1$
  }
}

Normally, the number of iterations required for convergence is much lesser than *n*, hence the cost of GMRES is dominated by the $O(n^2)$ operations of the matrix-vector product Ax^k in each iteration.

3. Pre-corrected FFT algorithm

The pFFT approach is used to improve the computational efficiency further by: (1) avoiding the formation of matrix A explicitly, and (2) approximating the matrix-vector product Ax^k in $O(n \log n)$ operations.

First, we divide the bounding region of our 3-D problem into $k \times l \times m$ array of small cells, so that each cell contains a number of panels. The idea of the pFFT approach is based on the fact that potentials at evaluation points far away from a cell can be accurately computed by representing the sources inside the cell by a small number of weighted point sources lying on a uniform grid. Furthermore, the computation of potentials on the uniform grid due to the grid sources is a discrete convolution, which can

be performed efficiently using FFT. The pFFT algorithm includes following steps:

(1) Project the panel sources onto a uniform grid of point sources.

(2) Compute the grid potentials due to the grid sources using FFT.

(3) Interpolate the grid potential onto the panels.

(4) Directly compute nearby interactions and pre-correction.

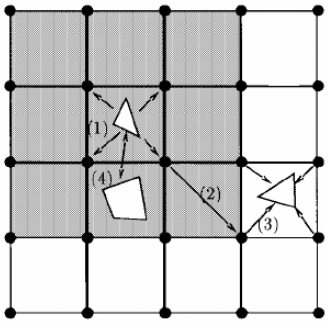

Fig. 1. Four steps of the pre-corrected FFT algorithm

Projection:

For each cell, we represent the given cell's source distribution with a small number ($p \times p \times p$) of weighted point sources on a uniform grid. One way to implement the projection step is that we choose a set of test points; at the test points, potentials due to the grid sources are forced to match the potentials due to the cell's source distribution.

This projection step will result a projection matrix [P]. And we have: $\bar{q}_g = [P]\bar{x}$

Convolution:

The grid potentials due to the grid sources can be computed by

$$\phi_{g,j} = \sum_i G(r_i, r_j) q_{g,i}$$

or in the matrix form

$$\bar{\phi}_g = [H]\bar{q}_g$$

where [H] is the convolution matrix. Since the Green's function is position invariant, we have

$$H_{ij} = G(r_i, r_j) = G(r_i - r_j, 0)$$

Matrix [H] is a multilevel Toeplitz matrix. It is well known that the Toeplitz matrix storage needs only $O(n)$ memory and a Toeplitz matrix-vector product can be computed in $O(n \log n)$ operations using FFT.

Interpolation:

Once the grid potentials have been computed, they must be interpolated onto the panels in each cell. The interpolation matrix [I] will be found. This process is similarly to the projection step.

$$\bar{\phi} = [I]\bar{\phi}_g$$

Direct matrix and pre-correction

From the above steps, we approximate matrix-vector product $\bar{\phi} = A\bar{x}$ by $\bar{\phi} = [I][H][P]\bar{x}$

This implies that we use the sparse representation of matrix A as: $A = [I][H][P]$. By doing this, we can reduce the memory storage and computation cost for matrix-vector product dramatically. However, the calculations of the potentials as above do not give accurate results for the nearby interactions. Therefore, we have to compute the nearby interactions directly and also remove the inaccurate contributions from the use of nearby grid sources.

Let i be the index of (source) panel charge, and N_i is the nearby neighbor set of ith source. The direct interactions between ith source and the list of nearby neighbors are computed as A_{ij} $(j \in N_i)$.

The pre-corrected direct matrix elements are then given by

$$D_{ij} = A_{ij} - [I^{(j)}][H^{(*)}][P^{(i)}]$$

It should be noted that N_i is a small set. Hence the pre-corrected direct matrix [D] is very sparse.

Implementation:

Part 1: Form the four matrices: [P], [H], [I], [D].

Part 2: Compute the matrix vector product: $y = Ax$.

$y_1 = [P]x$

$y_2 = fft(y_1)$

$y_3 = [H]y_2$

$y_4 = ifft(y3)$

$y_5 = [I]y_4$

$y = y_5 + [D]x$

4. Numerical Results

4.1 Drag force.

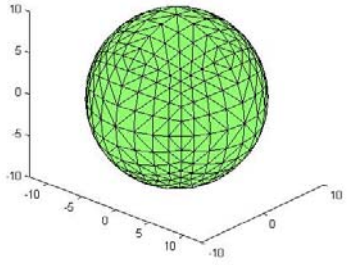

Fig. 2. The spherical paticle with 768 panels

We consider a particle in a cell-trap with fluid flowing at a velocity V_x = 1mm/s. The fluid medium is water ($\mu \approx 10^{-3} kg/ms$) and the particle has radius $R = 10\mu m$.

The Reynolds number is given by $\mathrm{Re} \approx 10^{-2} << 1$. We compute the force distribution q acting on the particle.The dense linear system is solved using GMRES in two different approaches: (i) direct calculation (forming matrix A, and doing matrix-vector product directly) and (ii) using pfft algorithm (approximating the matrix-vector product).

The total force F exerted on the particle is given by

$$F = -8\pi\mu \int_S q dS \ .$$

where q is the distributed force obtained from the BIE formulation. We compare the numerical result with the analytical solution from Stokes' drag law $F_d = -6\pi V \mu L$ (Fig. 3).

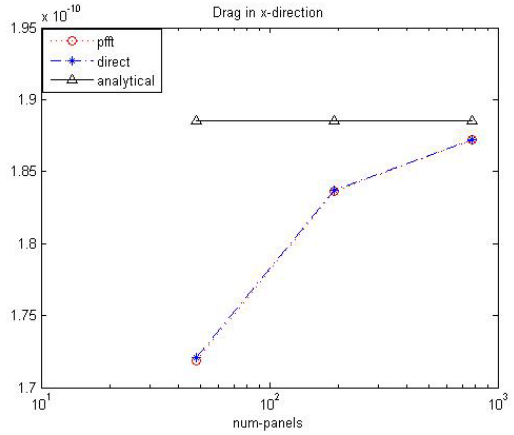

Fig. 3. Comparison of numerical results with analytical solution

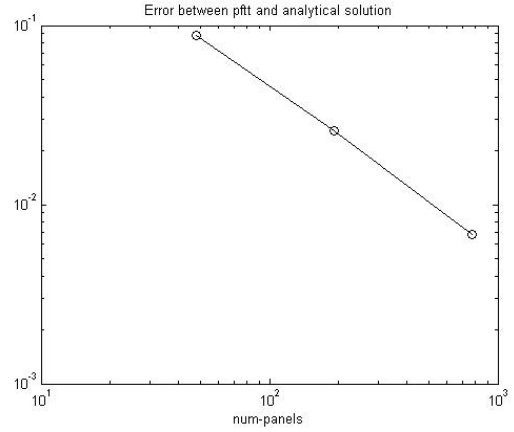

Fig. 4. Error from pFFT decreases with the number of panels.

The two approaches for solving dense linear system give very close results, which indicates that the pFFT algorithm can accurately approximate matrix-vector product. Also, the error between the numerical results and analytical solution decreases with the number of panels used.

4.2 DEP force

We consider a sphere in a quadrupole cell-trap as follows:

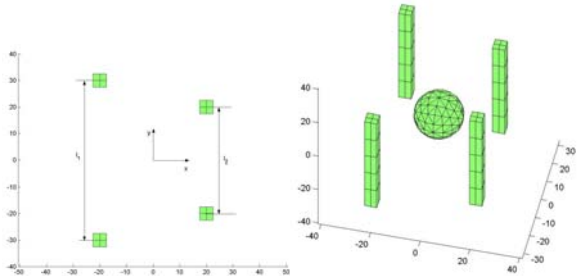

Fig. 5. Dimensions of the quadrupoles cell trap

The particle has radius $R = 10\mu m$ and dielectric permittivity $\varepsilon_p = 2$ .The fluid has permitivity $\varepsilon_f = 80$. The electrical potential barrier generated inside the trap is given in Fig. 6 and 7.

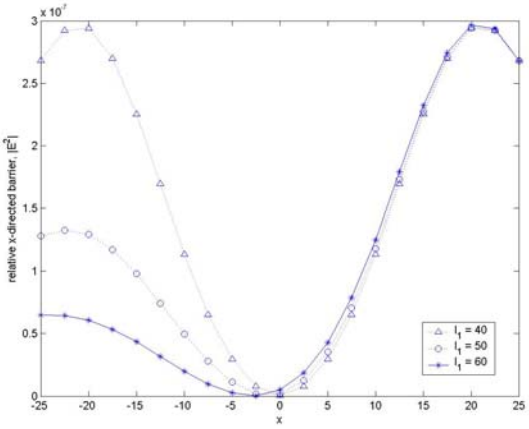

Fig. 6. The electric barrier is lowest at the center of the trap (applied voltage V = 1)

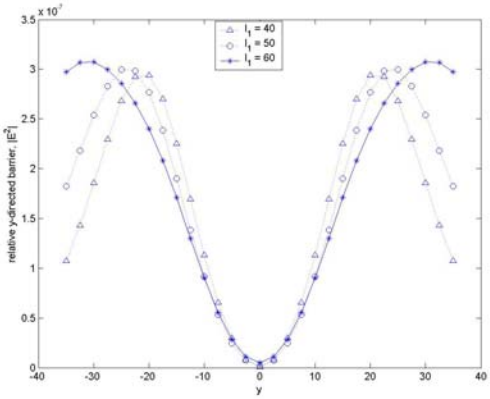

Fig. 7. y-directed electric barrier is symmetric and also lowest at the center of the trap

The electric potential barrier is lowest near the center of the trap. Since $\varepsilon_p < \varepsilon_f$, the particle is under the effect of negative DEP, and the stable position is near the center where field strength is lowest. The DEP force acting on the particle at different position is given in Fig. 8.

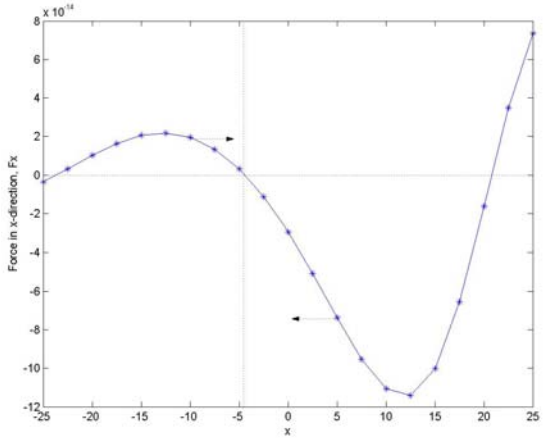

Fig. 8. DEP force acting on the particle in x-direction. Positive DEP force means positive direction of force.

The stable position is located near the center of the trap. Once the particle enters the trap from the left, the DEP force tends to pull the particle to the stable position. The steep force field "wall" on the right prevents the particle from escaping the trap. The equilibrium position of the particle is given by the position where the DEP force is balanced by the drag force from the surrounding fluid. By changing the applied voltages to the poles, and controlling the fluid flow rate through the trap, we can effectively manipulate the motion of the sphere.

Our numerical results above are quite close to some experimental results which given in [4] and [5].

5. Conclusions

We implemented the pFFT algorithm that improves the computational efficency of the BIE method while accurately approximating the matrix vector product. The method is used to solve both the electrostatic and Stokes flow problems. The numerical results are compared with analytical solution or experimental results, and the errors are found to be acceptable. From the results of forces (DEP force and Stokes' drag force) acting on a sphere, we can study the equilibrium position of the sphere in the cell trap, and also track its motion by forward integration in time.

The current study can be extended to arbitray shaped particles, possibly deformable, in the future. And an efficient algorithm, like pFFT, is crucial when such complex simulations are performed.

6. Acknowledgment

We would like to thank *pFFT group* at MIT (pfft@mit.edu) and Carlos Pinto Coelho for many helpful discussions and also for many helps in implementing pFFT.

References

[1] Joel R. Phillips, Jacob K. White, *A Precorrected-FFT Method for Electrostatic Analysis of Complicated 3-D Structure*, IEEE Vol. 16 (1997) 1059-1072.

[2] Zhenhai Zhu, Ben Song, Jacob White, *pfft++ - A general and extensible fast integral equation solver based on a pre-corrected FFT algorithm.*

[3] W. Ye, X. Wang, J. White, *A fast Stokes Solver for Generalized Flow Problems.*

[4] J.Voldman, M. Toner, M.L. Gray, M.A. Schmidt, *Design and analysis of extruded quadrupolar dielectrophoretic traps*, J. Electrostatic 57 (2003) 69-90.

[5] J.Voldman, Rebecca A. Braff, M. Toner, M.L. Gray, M.A. Schmidt, *Holding Forces of Single-Particle Dielectrophoretic Traps*, Biophysical Journal Vol. 80 (2001) 531-541.

[6] Carlos Rosales, Kian Meng Lim, *Numerical comparison between Maxwell stress method and equivalent multipole approach for calculation of the dielectrophoretic force in single-cell traps*, Electrophoresis (2005), 26, 2057-2065.

[7] C. A. Brebbia, S. Walker, *Boundary Element Techniques in Engineering*, Butterworth & Co. Ltd., 1980.

[8] C. Pozrikidis, *Boundary Integral and Singularity Methods for Linearized Viscous Flow*, Cambridge University Press 1992.