Fast Calculation of Hydrodynamic Interaction among Particles in the Stokes Flows

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1 INTRODUCTION

The aim of this work is to present an efficient computational method of hydrodynamic interaction among spherical particles in low-Reynolds-number flows. Stokesian Dynamics [1] has two major difficulties: the heavy computational load scaled by $O(N^3)$, and no systematic way to improve approximation. These will overcome by multipole expansion, iterative scheme, and fast multipole method.

2 MULTIPOLE EXPANSION

We use simple derivatives in Cartesian coordinate rather than harmonic functions in spherical coordinate.

Let us consider the many-body problem in the Stokes flow:

$$U_i(\boldsymbol{x}^\alpha) = \sum_\beta^N M_{ij}(\boldsymbol{x}^\alpha - \boldsymbol{y}^\beta) \cdot F_j(\boldsymbol{y}^\beta), \tag{1}$$

where $\boldsymbol{U}(\boldsymbol{x}^\alpha)$ is the velocity of particle α, $\boldsymbol{F}(\boldsymbol{y}^\beta)$ is the force of particle β to the fluid, and $\mathsf{M}(\boldsymbol{r})$ is the mobility matrix. Greek letters in upper-case are label of particle $(1, 2, \cdots, N)$ and Roman letters in lower-case are index of Cartesian coordinate (x, y, z). From the Taylor expansion with $\boldsymbol{y}^\beta$ at $\boldsymbol{y}_0$,

$$U_i(\boldsymbol{x}^\alpha) = \sum_{m=0}^p \mathcal{M}^m_{ij,k\cdots}(\boldsymbol{x}^\alpha - \boldsymbol{y}_0) \cdot \mathcal{F}^m_{jk\cdots}(\boldsymbol{y}_0), \tag{2}$$

where $\mathcal{M}^m$ is m-th order derivative of mobility matrix

$$\mathcal{M}^m_{ij,k\cdots}(\boldsymbol{r}) = \frac{1}{m!} \left(\frac{\partial}{\partial \boldsymbol{r}} \right)^m_{k\cdots} M_{ij}, \tag{3}$$

and $\mathcal{F}^m$ is m-th order force moment

$$\mathcal{F}^m_{jk\cdots}(\boldsymbol{y}_0) = \sum_\beta \left\{\boldsymbol{y}_0 - \boldsymbol{y}^\beta\right\}^m_{k\cdots} F_j(\boldsymbol{y}^\beta). \tag{4}$$

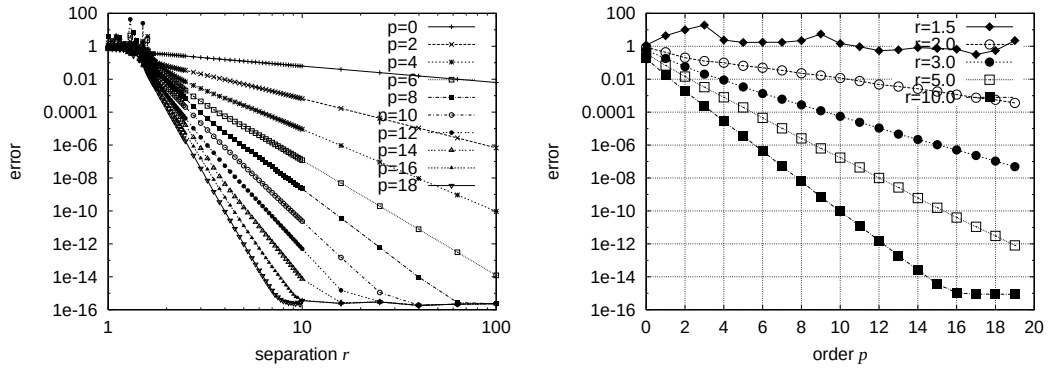

Figure 1: Error vs order p and separation r.

In Fig. 1, we consider two-body problems where particles are located at $\boldsymbol{x}$ and $\boldsymbol{y}$, under point-force approximation. The separation is defined by $r = |\boldsymbol{x}_0 - \boldsymbol{y}_0|$. The error $|\boldsymbol{U}_e - \boldsymbol{U}_d|/|\boldsymbol{U}_e|$ is averaged over 50 samples. $\boldsymbol{U}_d$ (direct) and $\boldsymbol{U}_e$ (expansion) are obtained by (1) and (2).

3 FAST CALCULATION

3.1 Iterative method

We need to calculate inverse in Stokesian Dynamics where resistance matrix R is approximated as

$$\mathsf{R} = \mathsf{M}^{-1} + \mathsf{L}. \tag{5}$$

where M is the mobility tensor with low order in expansion, and L is the lubrication tensor which contains contribution of higher order.

This inversion introduces many-body effect in way of method-of-reflections which is one of iterative method [2]. In turn, the application of iterative method which consists of the following matrix-vector product

$$\boldsymbol{U} = \mathsf{M} \cdot \boldsymbol{F} \tag{6}$$

is the first step to improve the calculation time which is scaled as $O(N^2)$.

3.2 Fast multipole expansion

Further improvement on speed is achieved on (6) in the iterative scheme by fast multipole method (FMM) [4]. The point of FMM is to expand not only with $\boldsymbol{y}$ but also with $\boldsymbol{x}$ in (1).

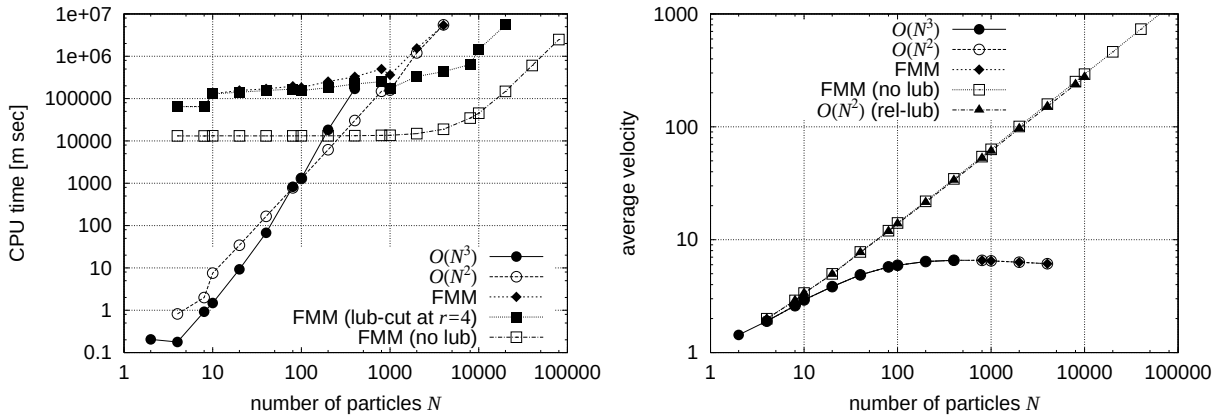

Figure 2: CPU time (left) and Average velocity (right).

Configuration of particles are regular array of simple-cubic lattice. In Fig. 2, $O(N^3)$ denots the original Stokesian Dynamics by (5), $O(N^2)$ denotes (5) using iterative method, FMM denotes (5) using iterative method with FMM, FMM(lub-cut) denotes FMM with cut-off in lubrication, FMM(no lub) denotes calculate without lubrication using FMM, and $O(N^2)$(rel-lub) denotes $O(N^2)$ using lubrication of relative motion. When $N < 100$, $O(N^3)$ is fastest, when $100 < N < 1000$, $O(N^2)$ is fastest, and when $1000 < N$, FMM(lub-cut) is fastest.

3.3 Systematic improvement of higher moments in Stokesian Dynamics

To improve accuracy, we need to improve base solution. For $\boldsymbol{x}_0 = \boldsymbol{y}_0$ (self-part),

$$\mathcal{U}^{(n)}_{i,l\cdots}(\boldsymbol{x}_0) = \sum_m \tilde{\mathcal{M}}^{(n,m)}_{i,l\cdots;j,k\cdots}\mathcal{F}^{(m)}_{j,k\cdots}(\boldsymbol{x}_0). \tag{7}$$

For $\boldsymbol{x}_0 \neq \boldsymbol{y}_0$,

$$\mathcal{V}^{(n)}_{i,l\cdots}(\boldsymbol{x}_0) = \sum_m \mathcal{M}^{(n,m)}_{i,l\cdots;j,k\cdots}(\boldsymbol{x}_0 - \boldsymbol{y}_0)\mathcal{F}^{(m)}_{j,k\cdots}(\boldsymbol{y}_0). \tag{8}$$

Relation between velocity derivatives and velocity moments are given by

$$\mathcal{U}^{(n)}_{i,l\cdots} = \sum_m \mathcal{V}^{(m)}_{i,k\cdots}\frac{1}{4\pi a^2}\int dS_r\ r^n_{l\cdots}r^m_{k\cdots} \tag{9}$$

Therefore, we get generalized grand mobility problem as

$$\begin{pmatrix} \boldsymbol{U} \\ \boldsymbol{\Omega} \\ \mathsf{E} \\ \hat{\mathcal{U}} \end{pmatrix} = \mathsf{M}\cdot\begin{pmatrix} \boldsymbol{F} \\ \boldsymbol{T} \\ \mathsf{S} \\ \hat{\mathcal{F}} \end{pmatrix}, \tag{10}$$

where $\boldsymbol{U}, \boldsymbol{\Omega}$ are translational and rotational velocity, E is asymmetric elements of first order (strain tensor), $\hat{\mathcal{U}}$ is irreducible velocity moments with higher moments, $\boldsymbol{F}, \boldsymbol{T}$ are force and torque, S is asymmetric elements of first order (stresslet tensor), and $\hat{\mathcal{F}}$ is irreducible force moments with higher moments.

We calculate mobility function of FTS versions – solving (10) under the condition of $\hat{\mathcal{U}} = 0$. (See Fig. 3.) FMM scheme of higher Stokesian Dynamics method Eq.(8), not Eq.(1), is also formulated.

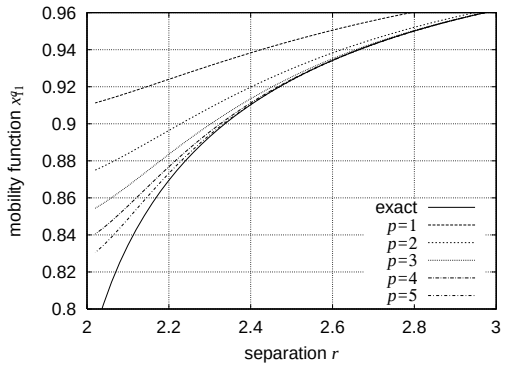

Figure 3: Mobility function x^a_{11}.

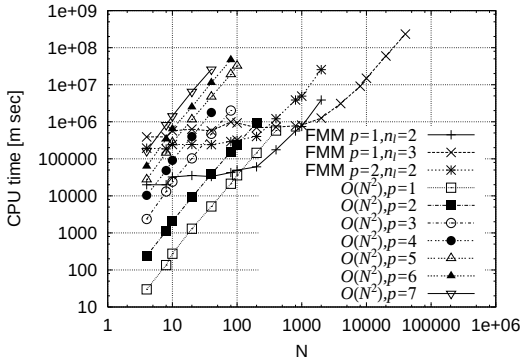

Figure 4: CPU time for higher SD method.

4 CONCLUSIONS

We established *FAST* and *ACCURATE* Stokesian Dynamics method. We have to give an explanation or proof for lubrication-correction, and formulate the case of periodic boundary condition.

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