Fast Calculation of Hydrodynamic Interaction among Particles in the Stokes Flows (粘性流体中の多粒子系の高速計算法)

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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:

1. the heavy computational load scaled by $O(N^3)$
2. no systematic way to improve approximation

These will overcome by

multipole expansion
iterative scheme
fast multipole method

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:

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

$\boldsymbol{U}(\boldsymbol{x}^\alpha)$: velocity of particle α
$\boldsymbol{F}(\boldsymbol{y}^\beta)$: force of particle β to the fluid
M($\boldsymbol{r}$) : the mobility matrix
Greek letter in upper-case : label of particle $(1, 2, \cdots, N)$
Roman letter in lower-case : 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

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

Results We consider two-body problems where particles are located at $\boldsymbol{x}$ and $\boldsymbol{y}$, under point-force approximation

$$M_{ij}(\boldsymbol{r}) = \frac{1}{r}\left(\delta_{ij} + \frac{r_i r_j}{r^2}\right). \tag{5}$$

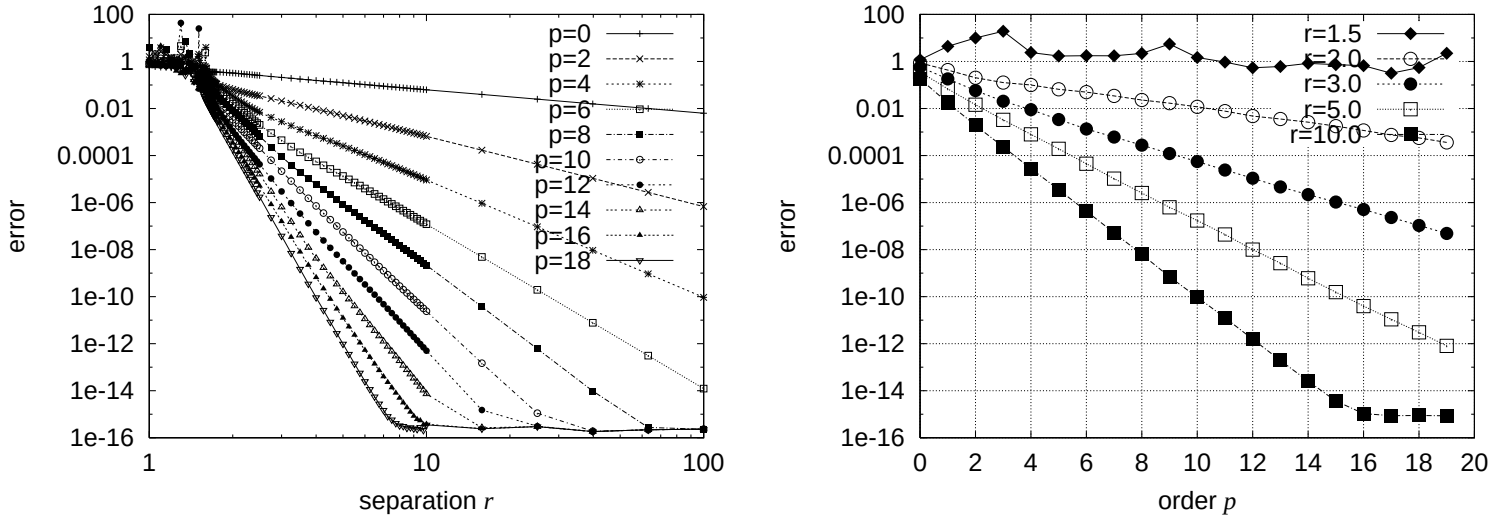

Figure 1 : Error vs order p and separation r.

The expansion-points $\boldsymbol{x}_0$ and $\boldsymbol{y}_0$ are located as

$$|\boldsymbol{x} - \boldsymbol{x}_0| = |\boldsymbol{y} - \boldsymbol{y}_0| = \sqrt{3}/2 \tag{6}$$

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)
Force on the particles are given as $\boldsymbol{F} = (1, 1, 1)$.

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

$$\mathsf{R} = \mathsf{M}^{-1} + \mathsf{L}. \tag{7}$$

M : mobility tensor with low order in expansion
L : 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

$$\boldsymbol{U} = \mathsf{M} \cdot \boldsymbol{F} \tag{8}$$

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

Fast multipole expansion Further improvement on speed is achieved on (8) 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).

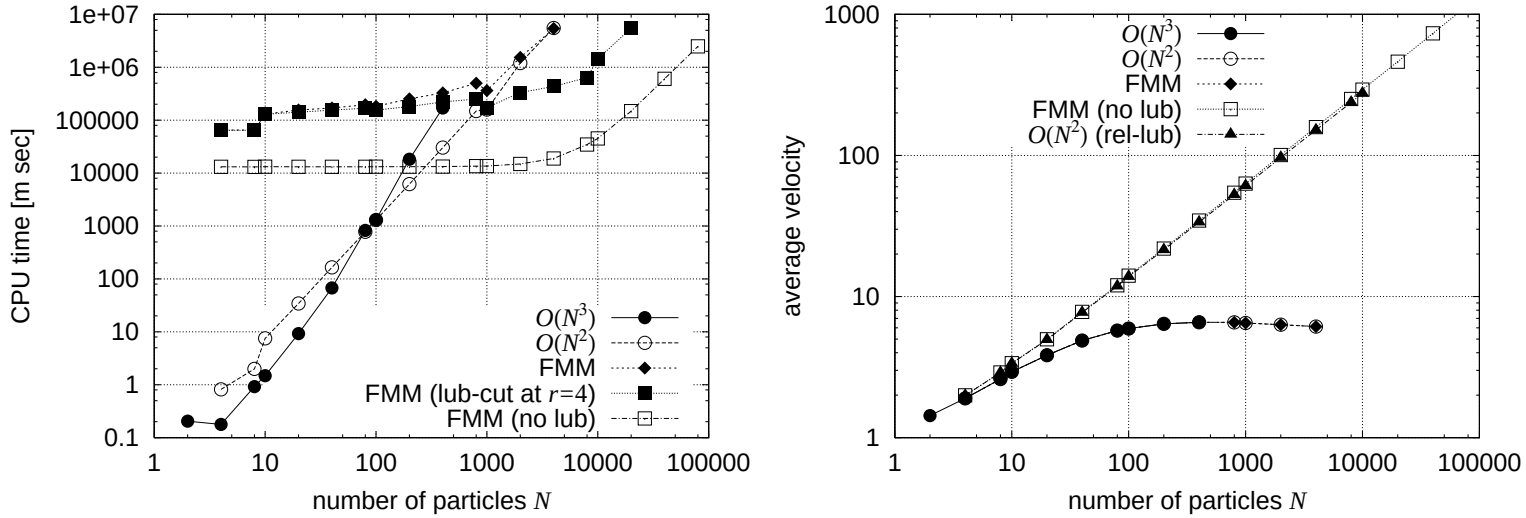

Figure 2 : CPU time (left) and Average velocity (right).

$O(N^3)$: the original Stokesian Dynamics by (7)
$O(N^2)$: (7) using iterative method called Orthomin
FMM : (7) using iterative method with FMM
FMM(lub-cut) : FMM with cut-off in lubrication
FMM(no lub) : calculate $\boldsymbol{U} = \mathrm{M} \cdot \boldsymbol{F}$ using FMM
$O(N^2)$(rel-lub) : $O(N^2)$ using lubrication of relative motion

Configuration of particles are regular array of simple-cubic lattice.

$N < 100$: $O(N^3)$ is fastest
$100 < N < 1000$: $O(N^2)$ is fastest
$1000 < N$: FMM(lub-cut) is fastest
(remark) FMM is comparable to $O(N^2)$ in $1000 < N$.)

It is expected that the average velocity is scaled as $N^{2/3}$
– FMM(no lub) and $O(N^2)$(rel-lub).

$O(N^3)$, $O(N^2)$, and FMM are wrong
– lubrication L in (7) may be wrong.

Excluding collective motion in lubrication [5] – $O(N^2)$(rel-lub) – helps this situation.

Systematic improvement of Stokesian Dynamics To improve accuracy, we need to improve base solution.

For $\boldsymbol{x}_0 = \boldsymbol{y}_0$ (self-part),

$$\mathcal{U}^{(n)}_{i,l\cdots}(\boldsymbol{x}_0) = \sum_m \tilde{\mathcal{M}}^{(n,m)}_{i,l\cdots;j,k\cdots} \mathcal{F}^{(m)}_{j,k\cdots}(\boldsymbol{x}_0), \tag{9}$$

where

$$\mathcal{U}^{(n)}_{i,l\cdots}(\boldsymbol{x}_0) = \frac{1}{4\pi a^2} \int dS_x \, \{\boldsymbol{x} - \boldsymbol{x}_0\}^n_{l\cdots} \, u_i(\boldsymbol{x}_0), \tag{10}$$

$$\tilde{\mathcal{M}}^{(n,m)}_{i,l\cdots;j,k\cdots} = \frac{1}{8\pi\mu} \frac{1}{m!} \frac{1}{4\pi a^2} \int dS_r \; r^m_{l\cdots} \left[\left(\frac{\partial}{\partial \boldsymbol{r}} \right)^n_{l\cdots} \left(\frac{\partial}{\partial \boldsymbol{r}} \right)^m_{k\cdots} J_{ij} \right] (\boldsymbol{r}). \tag{11}$$

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

$$\mathcal{V}^{(n)}_{i,l\cdots}(\boldsymbol{x}_0) = \sum_m \mathcal{M}^{(n,m)}_{i,l\cdots;j,k\cdots}(\boldsymbol{x}_0 - \boldsymbol{y}_0)\mathcal{F}^{(m)}_{j,k\cdots}(\boldsymbol{y}_0), \tag{12}$$

where $\mathcal{V}^{(n)}$ is n-th order velocity derivative defined by

$$\mathcal{V}^{(n)}_{i,l\cdots}(\boldsymbol{x}) = \frac{1}{n!}\left[\left(\frac{\partial}{\partial \boldsymbol{r}}\right)^n_{l\cdots} u_i\right](\boldsymbol{x}), \tag{13}$$

$$\mathcal{M}^{(n,m)}_{i,l\cdots;j,k\cdots}(\boldsymbol{r}) = \frac{1}{n!m!}\left[\left(\frac{\partial}{\partial \boldsymbol{r}}\right)^n_{l\cdots}\left(\frac{\partial}{\partial \boldsymbol{r}}\right)^m_{k\cdots} J_{ij}\right](\boldsymbol{r}). \tag{14}$$

Relation between velocity derivatives and velocity moments are given by

$$\mathcal{U}^{(n)}_{i,l\cdots} = \sum_m \mathcal{V}^{(m)}_{i,k\cdots}\frac{1}{4\pi a^2}\int dS_r \; r^n_{l\cdots} r^m_{k\cdots} \tag{15}$$

$$\begin{pmatrix} \boldsymbol{U} \\ \boldsymbol{\Omega} \\ \mathsf{E} \\ \hat{\mathcal{U}} \end{pmatrix} = \mathsf{M} \cdot \begin{pmatrix} \boldsymbol{F} \\ \boldsymbol{T} \\ \mathsf{S} \\ \hat{\mathcal{F}} \end{pmatrix}, \tag{16}$$

Vector in left-hand-side is irreducible velocity moments
$\boldsymbol{U}, \boldsymbol{\Omega}$: translational and rotational velocity
E : asymmetric elements of first order (strain tensor)
$\hat{\mathcal{U}}$: irreducible velocity moments with higher moments

Vector in right-hand-side is irreducible force moments
$\boldsymbol{F}, \boldsymbol{T}$: force and torque
S : asymmetric elements of first order (stresslet tensor)
$\hat{\mathcal{F}}$: irreducible force moments with higher moments

Check We calculate mobility function of FTS versions – solving (16) under the condition of $\widehat{\mathcal{U}} = 0$.

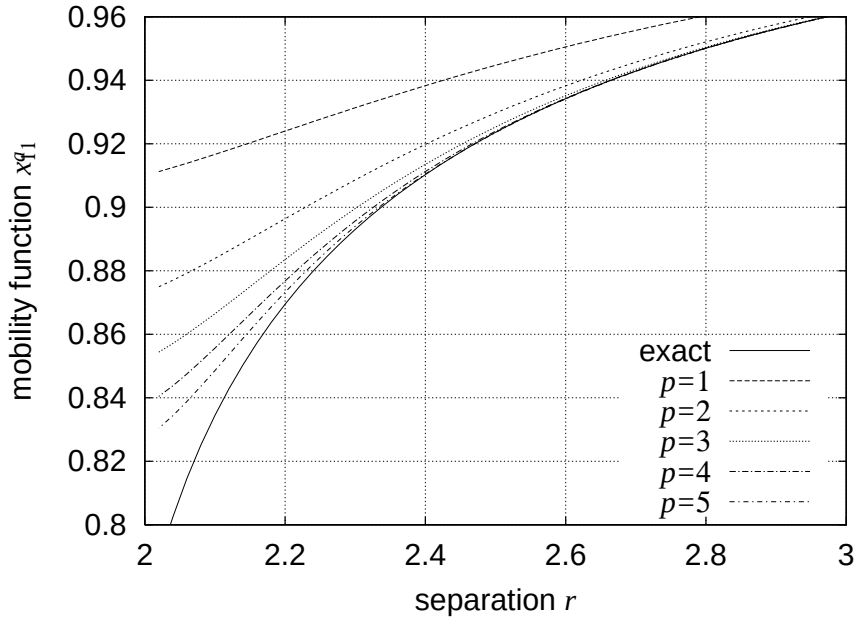

Figure 3 : Mobility function x^a_{11}.

FMM scheme of higher Stokesian Dynamics method Eq.(12), not Eq.(1), is also formulated.

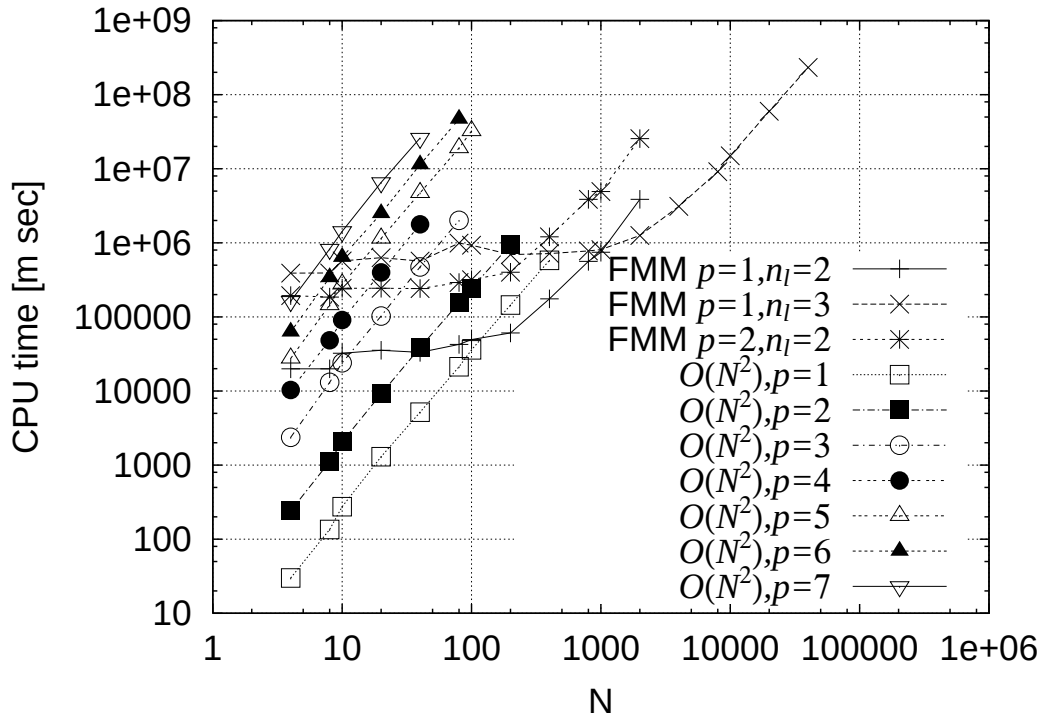

Figure 4 : CPU time for higher SD method.

Conclusions

- established FAST and ACCURATE Stokesian Dynamics method!

Discussions

- give an explanation or proof for lubrication-correction

- formulate the case of periodic boundary condition

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