# 粘性流の粒子間相互作用の高速、高精度数値計算法

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## 1 Introduction

Microstructure of suspensions have been attracting many attentions of researchers in physics and chemical engineering. Stokesian Dynamics method has developed for many-particle system first under the free boundary condition by [6] and shortly extended to that under the periodic boundary condition by [2] (see also [1]).

Although the Stokesian Dynamics method was successful in some respect, recently two major difficulties are recognized. One is its heavy calculation, because of which the size of the system to simulate is limited around a few hundred particles, and the other is the limitation of its approximation up to so-called $FTS$ version where only force, torque and stresslet are considered and higher force moments are neglected in the multipole expansion of the velocity.

In this work we consider rigid spherical particles under the free boundary condition where Brownian motion and inertial effects of fluid are negligible; that is, Peclet number is infinite and particle Reynolds number is zero. The main purpose of this work is to establish the formulation and the implementation into the numerical schemes, so that the applications for interesting phenomena are outside of the scope.

## 2 Multipole expansion

### 2.1 Expansion of velocity field

Velocity disturbance $\boldsymbol{v}(\boldsymbol{x})$ caused by rigid particles is written by so-called single-layer potentials ([14]) as

$$v_i(\boldsymbol{x}) = u_i(\boldsymbol{x}) - u_i^{\infty}(\boldsymbol{x}) = -\frac{1}{8\pi\mu}\sum_{\alpha=1}^{N}\int_{S_\alpha} dS(\boldsymbol{y})\ J_{ij}(\boldsymbol{x}-\boldsymbol{y})f_j(\boldsymbol{y}), \tag{1}$$

where $N$ is the number of particles, $S_\alpha$ is the surface of particle $\alpha$, $\boldsymbol{u}$ is the fluid velocity, $\boldsymbol{u}^\infty$ is the velocity in case without particles, $\mu$ is the viscosity of the fluid, $\boldsymbol{f}$ is force density on the surface $\boldsymbol{y}$, and $\mathsf{J}(\boldsymbol{r})$ is Oseen tensor given by

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

We adopt the Einstein convention for repeated indices throughout this paper. We can expand $\boldsymbol{y}$ in the right-hand-side of (1) at the centre of particle $\boldsymbol{x}^\alpha$ as

$$v_i(\boldsymbol{x}) = \sum_{\alpha=1}^{N} \sum_{m=0}^{p'} \mathcal{J}^{(m)}_{ij,k\cdots}(\boldsymbol{x} - \boldsymbol{x}^\alpha)\mathcal{F}^{(m)}_{j,k\cdots}(\alpha), \tag{3}$$

where $p'$ is the order of truncation (discussed in detail in §2.4), $\mathcal{F}^{(m)}_{j,k\cdots}(\alpha)$ is the force moment of particle $\alpha$ defined by

$$\mathcal{F}^{(m)}_{j,k\cdots}(\alpha) = -\int_{S_\alpha} dS(\boldsymbol{y})\ (\boldsymbol{y} - \boldsymbol{x}^\alpha)^m_{k\cdots} f_j(\boldsymbol{y}), \tag{4}$$

and

$$\mathcal{J}^{(m)}_{ij,k\cdots}(\boldsymbol{r}) = \frac{1}{8\pi\mu}\frac{1}{m!}\left[(-\nabla)^m_{k\cdots}\, J_{ij}\right](\boldsymbol{r}). \tag{5}$$

## 2.2 Boundary conditions

We introduce $\boldsymbol{f}$ in (1) or $\mathcal{F}$ in (3) as a parameter to match the boundary conditions for the velocity. In order to specify all elements of $\mathcal{F}$ in (3), we need the same number of boundary conditions on the velocity. There are, at least, three approaches; the boundary collocation method, the method using velocity derivatives, and the method using velocity moments.

In the boundary collocation method by [7], we directly apply the boundary conditions on a finite number of points on the surface called the collocation points. Another way is to consider velocity derivatives $\mathcal{V}$ at the centre of particle defined by

$$\mathcal{V}^{(n)}_{i,l\cdots}(\boldsymbol{x}^\alpha) = \frac{1}{n!}\left[\nabla^n_{l\cdots} v_i\right](\boldsymbol{x}^\alpha). \tag{6}$$

This approach is also simple, however, the velocity derivatives $\mathcal{V}$ have two disadvantages; the symmetry is different from that of the force moments $\mathcal{F}$, and the velocity derivatives for the self part becomes singular in the expansion (3).

As the other way, we introduce velocity moments $\mathcal{U}$ defined by

$$\mathcal{U}^{(n)}_{i,l\cdots}(\alpha) = \frac{1}{4\pi a^2}\int_{S_\alpha} dS(\boldsymbol{y})\,(\boldsymbol{y} - \boldsymbol{x}^\alpha)^n_{l\cdots}\, v_i(\boldsymbol{y}), \tag{7}$$

where $a$ is the radius of particles. The velocity moments $\mathcal{U}$ are more complicated than the velocity derivatives $\mathcal{V}$, but the two difficulties are completely overcome. The velocity at the surface is given by $\boldsymbol{v}(\boldsymbol{y}) = \boldsymbol{U}^\alpha + \boldsymbol{\Omega}^\alpha \times (\boldsymbol{y} - \boldsymbol{x}^\alpha) + \mathsf{E}^\alpha \cdot (\boldsymbol{y} - \boldsymbol{x}^\alpha)$, where $\boldsymbol{U}^\alpha$, $\boldsymbol{\Omega}^\alpha$, and $\mathsf{E}^\alpha$ are the translational velocity, the angular velocity, and the rate of strain for particle $\alpha$ relative to the imposed flow $\boldsymbol{u}^\infty$.

The linear set of equations relating the velocity moments and the force moments are obtained by applying the surface integral in (7) for (3) as

$$\mathcal{U}^{(n)}_{i,l\cdots}(\alpha) = \sum_{\beta=1}^{N} \sum_{m=0}^{p'} \mathcal{M}^{(n,m)}_{i,l\cdots;j,k\cdots}(\alpha,\beta) \mathcal{F}^{(m)}_{j,k\cdots}(\beta), \tag{8}$$

where

$$\mathcal{M}^{(n,m)}_{i,l\cdots;j,k\cdots}(\alpha,\beta) = \frac{1}{4\pi a^2} \int_{S_\alpha} dS(\boldsymbol{y}) \ (\boldsymbol{y} - \boldsymbol{x}^\alpha)^n_{l\cdots} \mathcal{J}^{(m)}_{ij,k\cdots}(\boldsymbol{y} - \boldsymbol{x}^\beta). \tag{9}$$

We call (8) or in the abbreviate form

$$\mathcal{U} = \mathcal{M} \cdot \mathcal{F} \tag{10}$$

as the generalized mobility problem and the matrix $\mathcal{M}$ as the generalized mobility matrix. In the following we often omit indices and arguments in this way, just for simplicity.

For the practical calculation of the generalized mobility problem which is the main aim of this work, we split the velocity moments $\mathcal{U}$ into two parts – self part $\mathcal{U}^s$ and non-self part $\mathcal{U}'$ as

$$\mathcal{U} = \mathcal{U}^s + \mathcal{U}'. \tag{11}$$

This is because $\mathcal{J}$ is much easier than $\mathcal{M}$ to calculate. The self part $\mathcal{U}^s$ is written as

$$\mathcal{U}^s = \mathcal{M}^s \cdot \mathcal{F}, \tag{12}$$

where the self part of the mobility matrix $\mathcal{M}^s$ is given by

$$\mathcal{M}^{s\,(n,m)}_{i,l\cdots;j,k\cdots} = \mathcal{M}^{(n,m)}_{i,l\cdots;j,k\cdots}(\alpha,\alpha) = \frac{1}{4\pi a^2} \int_{|\boldsymbol{r}|=a} dS(\boldsymbol{r}) \ r^n_{l\cdots} \mathcal{J}^{(m)}_{ij,k\cdots}(\boldsymbol{r}). \tag{13}$$

It is found that $\mathcal{M}^{s\,(n,m)}$ has the following properties: (i) it is non-zero only when $n$ and $m$ are both odd or both even, and (ii) it is zero for $m \geq n+2$. For the non-self part, it is convenient to consider the relation between velocity moments $\mathcal{U}'$ and velocity derivatives $\mathcal{V}'$ where dash denotes the non-self part. First we define the non-self part of the velocity disturbance caused by particles $\beta \neq \alpha$ as

$$v'^{\alpha}_{i}(\boldsymbol{x}) = \sum_{\beta\neq\alpha} \sum_{m=0}^{p'} \mathcal{J}^{(m)}_{ij,k\cdots}(\boldsymbol{x} - \boldsymbol{x}^\beta) \mathcal{F}^{(m)}_{j,k\cdots}(\beta), \tag{14}$$

and the non-self part of the velocity derivatives $\mathcal{V}'$ as

$$\mathcal{V}'^{(m)}(\alpha) = \frac{1}{m!}\left[\nabla^m v'^{\alpha}_i\right](\boldsymbol{x}^\alpha). \tag{15}$$

Expanding the velocity $\boldsymbol{v}'^{\alpha}$ at the centre $\boldsymbol{x}^\alpha$ as

$$v'^{\alpha}_i(\boldsymbol{y}) = \sum_{m=0} \mathcal{V}'^{(m)}_{i,k\cdots}(\alpha)\,(\boldsymbol{y}-\boldsymbol{x}^\alpha)^m_{k\cdots}\,, \tag{16}$$

the non-self part of the velocity moment for particle $\alpha$ is written by that of the velocity derivatives as

$$\mathcal{U}'^{(n)}_{i,l\cdots}(\alpha) = \sum_{m=0}^{n+2} \mathcal{V}'^{(m)}_{i,k\cdots}(\alpha)\frac{1}{4\pi a^2}\int_{S_\alpha} dS(\boldsymbol{y})\ \ (\boldsymbol{y}-\boldsymbol{x}^\alpha)^{n+m}_{l\cdots k\cdots}\,. \tag{17}$$

## 2.3 Reduction of moments

When we need to solve some elements of the force moments by the other force moments and appropriate elements of the velocity moments, we should reduce the degrees of freedom. The reduction related to the nature of the velocity field itself – the incompressibility and the biharmonic nature – are already discussed in §2.2. There is another dependence among elements of the moments from the nature of spherical particles.

For velocity moments $\mathcal{U}^{(m)}_{i,k\cdots}$, there is obvious symmetry of indices $k\cdots$. From this symmetry, independent number of elements at $m$th order becomes $(m+1)(m+2)/2$. We call the form of this reduction as the 'symmetric form'.

From the definition of the moments, the higher rank depends on the lower rank in the way of

$$\mathcal{U}^{(n+2)}_{j,ssk\cdots} = a^2\mathcal{U}^{(n)}_{j,k\cdots}. \tag{18}$$

To reduce this dependence, it is convenient to introduce the irreducible tensor which is symmetric and traceless. The reduction for a $p$-rank tensor $A^p_{i\cdots}$ is given by [5] as

$$\hat{A}^p_{i\cdots} = \sum_{k=0}^{[p/2]} a^p_k \delta_{(i_1 i_2}\delta_{i_3 i_4}\cdots\delta_{i_{2k-1}i_{2k}}A^p_{i_{2k+1}\cdots i_p)s_1 s_1\cdots s_k s_k}\,, \tag{19}$$

where

$$a^p_k = (-1)^k\frac{p!}{(p-2k)!}\frac{(2p-2k-1)!!}{(2p-1)!!(2k)!!}. \tag{20}$$

For example, we have the following relations for $p = 2$ and 3;

$$\hat{A}^2_{ij} = A^2_{(ij)} - \frac{1}{3}\delta_{ij}A^2_{ss}, \tag{21}$$

and

$$\hat{A}^3_{ijk} = A^3_{(ijk)} - \frac{1}{5}\left(\delta_{ij}A^3_{(kss)} + \delta_{jk}A^3_{(iss)} + \delta_{ki}A^3_{(jss)}\right). \tag{22}$$

The parentheses around the indices in (19) indicate the symmetrization for the indices. For the moments in our case, the indices are symmetric by the definition, so that we do not need to care about the symmetrization. By this reduction, the number of independent elements on $m$th order becomes $2m+1$.

We write this reduction operator as $\mathcal{P}$ and the inverse operator (recovery operator) as $\mathcal{Q}$. By these operators, irreducible moments $\hat{\mathcal{U}}$ and $\hat{\mathcal{F}}$ are related as

$$\hat{\mathcal{U}} = \mathcal{P}\cdot\mathcal{M}\cdot\mathcal{Q}\cdot\hat{\mathcal{F}}, \tag{23}$$

which we call the irreducible generalized mobility problem. The concrete procedure to calculate (23) is discussed in §2.4 and the application of the boundary conditions for it is discussed in §2.5.

## 2.4 Truncation

The truncation implicitly introduced in (3) should be considered on the irreducible form (23) where the independent elements are explicitly specified; that is, we introduce the order of truncation $p$ as the maximum order of $\hat{\mathcal{U}}$ and $\hat{\mathcal{F}}$ in (23).

The practical calculation of (23) is given as the following six-step procedure for particles $\alpha = 1, \cdots, N$ where we write the order of truncation $p$ explicitly:

i. Recover the force moments $\mathcal{F}$ by the irreducible force moments $\hat{\mathcal{F}}$ as the input by

$$\begin{bmatrix} \mathcal{F}^{(0)} \\ \vdots \\ \mathcal{F}^{(p)} \\ \mathcal{F}^{(p+1)} \\ \mathcal{F}^{(p+2)} \end{bmatrix}(\alpha) = \begin{bmatrix} \mathcal{Q}^{(0,0)} & \cdots & \mathcal{Q}^{(0,p)} \\ \vdots & \ddots & \vdots \\ \mathcal{Q}^{(p,0)} & \cdots & \mathcal{Q}^{(p,p)} \\ \mathcal{Q}^{(p+1,0)} & \cdots & \mathcal{Q}^{(p+1,p)} \\ \mathcal{Q}^{(p+2,0)} & \cdots & \mathcal{Q}^{(p+2,p)} \end{bmatrix} \cdot \begin{bmatrix} \hat{\mathcal{F}}^{(0)} \\ \vdots \\ \hat{\mathcal{F}}^{(p)} \end{bmatrix}(\alpha). \tag{24}$$

ii. Calculate the non-self part of the velocity derivatives $\mathcal{V}'$ from $\mathcal{F}$ by

$$\begin{bmatrix} \mathcal{V}'^{(0)} \\ \vdots \\ \mathcal{V}'^{(p+2)} \end{bmatrix}(\alpha) = \sum_{\beta\neq\alpha} \begin{bmatrix} \mathcal{K}^{(0,0)} & \cdots & \mathcal{K}^{(0,p+2)} \\ \vdots & \ddots & \vdots \\ \mathcal{K}^{(p+2,0)} & \cdots & \mathcal{K}^{(p+2,p+2)} \end{bmatrix}(\boldsymbol{x}^\alpha - \boldsymbol{y}^\beta)\cdot \begin{bmatrix} \mathcal{F}^{(0)} \\ \vdots \\ \mathcal{F}^{(p+2)} \end{bmatrix}(\beta), \tag{25}$$

where

$$\mathcal{K}^{(n,m)}_{i,l\cdots;j,k\cdots}(\boldsymbol{r}) = \frac{1}{n!}\left[\nabla^n_{l\cdots}\mathcal{J}^{(m)}_{ij,k\cdots}\right](\boldsymbol{r}) = \frac{1}{8\pi\mu}\frac{1}{n!}\frac{1}{m!}\left[\nabla^n_{l\cdots}(-\nabla)^m_{k\cdots}J_{ij}\right](\boldsymbol{r}). \tag{26}$$

iii. Convert the velocity derivatives $\mathcal{V}'$ to the velocity moments $\mathcal{U}'$ by (17) as

$$\begin{bmatrix} \mathcal{U}'^{(0)} \\ \vdots \\ \mathcal{U}'^{(p)} \end{bmatrix}(\alpha) = \begin{bmatrix} \mathcal{D}^{(0,0)} & \cdots & \mathcal{D}^{(0,p)} & \mathcal{D}^{(0,p+1)} & \mathcal{D}^{(0,p+2)} \\ \vdots & \ddots & \vdots & \vdots & \vdots \\ \mathcal{D}^{(p,0)} & \cdots & \mathcal{D}^{(p,p+2)} & \mathcal{D}^{(p,p+1)} & \mathcal{D}^{(p,p+2)} \end{bmatrix} \cdot \begin{bmatrix} \mathcal{V}'^{(0)} \\ \vdots \\ \mathcal{V}'^{(p)} \\ \mathcal{V}'^{(p+1)} \\ \mathcal{V}'^{(p+2)} \end{bmatrix}(\alpha), \quad (27)$$

where

$$\mathcal{D}^{(n,m)} = \frac{a^{n+m}}{4\pi} \int_{|\hat{\boldsymbol{r}}|=1} dS(\hat{\boldsymbol{r}})\ \hat{\boldsymbol{r}}^{n+m}. \quad (28)$$

iv. Calculate the self part of the velocity moment $\mathcal{U}^s$ by

$$\begin{bmatrix} \mathcal{U}^{s(0)} \\ \vdots \\ \mathcal{U}^{s(p)} \end{bmatrix}(\alpha) = \begin{bmatrix} \mathcal{M}^{s(0,0)} & \cdots & \mathcal{M}^{s(0,p)} \\ \vdots & \ddots & \vdots \\ \mathcal{M}^{s(p,0)} & \cdots & \mathcal{M}^{s(p,p)} \end{bmatrix} \cdot \begin{bmatrix} \mathcal{F}^{(0)} \\ \vdots \\ \mathcal{F}^{(p)} \end{bmatrix}(\alpha), \quad (29)$$

where $\mathcal{M}^s$ is given by (13).

v. Calculate the velocity moments $\mathcal{U}$ summing the self part and the non-self part as

$$\begin{bmatrix} \mathcal{U}^{(0)} \\ \vdots \\ \mathcal{U}^{(p)} \end{bmatrix}(\alpha) = \begin{bmatrix} \mathcal{U}^{s(0)} \\ \vdots \\ \mathcal{U}^{s(p)} \end{bmatrix}(\alpha) + \begin{bmatrix} \mathcal{U}'^{(0)} \\ \vdots \\ \mathcal{U}'^{(p)} \end{bmatrix}(\alpha). \quad (30)$$

vi. Reduce the velocity moments $\mathcal{U}$ into $\hat{\mathcal{U}}$ as

$$\begin{bmatrix} \hat{\mathcal{U}}^{(0)} \\ \vdots \\ \hat{\mathcal{U}}^{(p)} \end{bmatrix}(\alpha) = \begin{bmatrix} \mathcal{P}^{(0,0)} & \cdots & \mathcal{P}^{(0,p)} \\ \vdots & \ddots & \vdots \\ \mathcal{P}^{(p,0)} & \cdots & \mathcal{P}^{(p,p)} \end{bmatrix} \cdot \begin{bmatrix} \mathcal{U}^{(0)} \\ \vdots \\ \mathcal{U}^{(p)} \end{bmatrix}(\alpha). \quad (31)$$

The above six-step procedure as a whole could be recognized as a subroutine of (23) which has the irreducible force moment $\hat{\mathcal{F}}$ as the input and returns the irreducible velocity moment $\hat{\mathcal{U}}$.

It should be noted that even in the truncation at order $p$ on $\hat{\mathcal{F}}$ and $\hat{\mathcal{U}}$ in (23), we have to recover force moments up to order $p+2$, calculate the velocity derivatives with order $p+2$, and then, convert them into the velocity moments with order $p$. Therefore the truncation order $p'$ in (3), (8), and (14), is $p+2$.

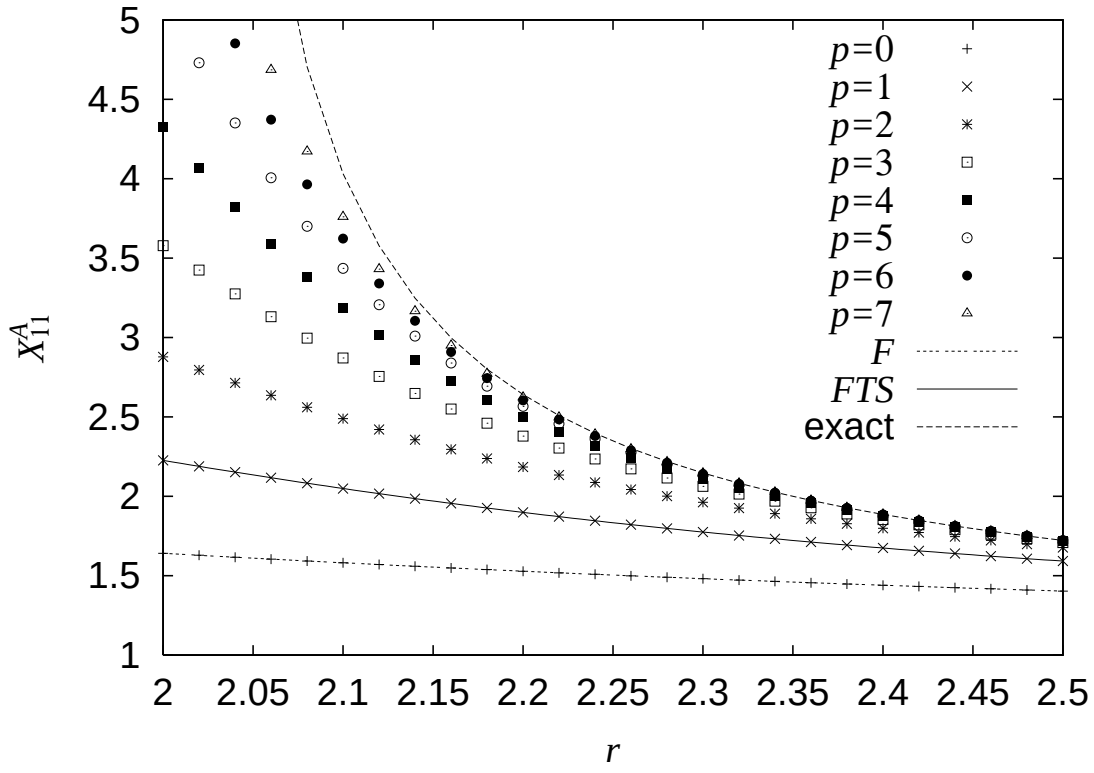


Figure 1: The scalar function $X_{11}^A(r)$ of the two-body resistance problem for various case. '$F$' and '$FTS$' show the corresponding values obtained by the analytical expressions and 'exact' shows the results by Jeffrey & Onishi (1984). The results by the present formulation are shown as $p = 0, 1, \cdots, 7$.

### 2.5 Higher version for rigid particles

For the check of the formulation and the implementation, we calculate the two-body resistance matrix for $p = 0, 1, \cdots, 7$ and compare them to the exact solution by [11]. In addition, we can compare the results with the analytical forms of the scalar functions. Figure 1 shows one of the scalar functions in the resistance matrix $X_{11}^A(r)$ for various cases. The analytical expression of $X_{11}^A(r)$ for $F$ version is given by

$$X_{11}^A(r) = \frac{4r^6}{4r^6 - (3r^2 - 2)^2}, \tag{32}$$

and for $FTS$ version is given by

$$X_{11}^A(r) = \frac{20r^6}{D}\left(-2880 + 2208r^2 - 260r^4 - 75r^6 + 20r^{10}\right), \tag{33}$$

where

$$\begin{aligned} D &= 2304 - 21120r^2 + 55600r^4 - 90600r^6 + 45945r^8 \\ &\quad -800r^{10} - 1800r^{12} - 900r^{14} + 400r^{16}. \end{aligned} \tag{34}$$

This shows that the results of $p = 0$ and $p = 1$ are completely identical to the analytical results and converge to the exact solution as $p \to \infty$.

## 3 Fast scheme

The bottleneck in the Stokesian Dynamics method is in the inversion of the mobility matrix. Therefore we need to improve the calculation of the linear set of equations faster than $O(N^3)$. As suggested by [10], the application of conjugate-gradient type iterative methods is the first step for the improvement. The iterative method for the Stokesian Dynamics method gives an $O(N^2)$ scheme at best, consisting only of the calculation of the dot-product between the mobility matrix and the force moment, which would be the next bottleneck. The fast multipole method, which is a simple extension of the conventional multipole expansion, is applicable for the calculation and gives an $O(N)$ scheme with a good convergence.

Before proceeding we consult the cost of calculation in the six-step procedure to see where the next bottleneck is. The steps except for (ii) are the calculation for each particles, and therefore the cost is $O(N)$. On the other hand, the calculation of the step (ii) contains the summation for $N - 1$ particles, so that the cost is $O(N^2)$, which is the current bottleneck.

## 3.1 Fast multipole method – $O(N)$ scheme

FMM is originally developed by [8] for Laplace problem in two- and three-dimensions with non-adaptive tree-structure, and is extended shortly to adaptive one by [3]. The application to the low-Reynolds-number flows is shown by [19]. The aim of our formulation of FMM is to make the scheme for free boundary condition with a simple formulation, while [19]'s formulation is for periodic boundary condition and is so complicated. We only consider the non-adaptive scheme in this work.

### 3.1.1 Outline of FMM

Our aim is now to calculate $\mathcal{V}'(\alpha)$ defined by (25) efficiently. The point of FMM is that we treat particles as a group not only for $\beta$'s in the force moments $\mathcal{F}(\beta)$ but also for $\alpha$'s in the velocity derivatives $\mathcal{V}'(\alpha)$ in (25). In other words, we expand not only $\boldsymbol{y}$ but also $\boldsymbol{x}$ on the integral equation (1).

To make an efficient procedure to calculate the velocity derivatives, we introduce hierarchical cell-structure and formulate the calculations between the levels of the cell-structure. First we define the primary cell at level 0 which contains all particles. At the next level 1, we divide the primary cell into $2^3$ cells called '*children*.' This division is repeated up to the level $l_m$, where the cells are called '*leaves*'. All cells except for leaves have 8 children and all cells except for the primary cell have their '*parent*' cell.

First we are going to formulate the basic formulae to shift the origin of the force moments and that of the velocity derivatives, and then, to discuss the concrete implementation of FMM.

### 3.1.2 Shift-operation of force moments

We describe the transformations of the origin of moments here. We would like to represent the moments with the origin $\boldsymbol{x}_2$ by $\mathcal{F}(\boldsymbol{x}_1)$. From the definition, the moments with $\boldsymbol{x}_2$ is given by

$$\mathcal{F}^{(m)}_{i,k\cdots}(\boldsymbol{x}_2) = \int dS(\boldsymbol{y})\ \ (\boldsymbol{y}-\boldsymbol{x}_2)^m_{k\cdots}\, f_i(\boldsymbol{y})\,. \tag{35}$$

Here $(\boldsymbol{y}-\boldsymbol{x}_2)^m$ could be written by the linear combination of $(\boldsymbol{y}-\boldsymbol{x}_1)^i$ and $(\boldsymbol{x}_1-\boldsymbol{x}_2)^j$ where $i+j=m$. By the 'binomial theorem for 3-dimensional vectors', we are able to transform $\mathcal{F}(\boldsymbol{x}_1)$ to $\mathcal{F}(\boldsymbol{x}_2)$ uniquely. The point of the binomial theorem for vectors is the non-commutable property;

$$a_i b_j \neq b_i a_j. \tag{36}$$

The expansion of power of the sum of two vectors $\boldsymbol{a}$ and $\boldsymbol{b}$ is, though, straightforward. We just write down explicitly for lower powers;

$$\mathcal{F}^{(0)}_i(\boldsymbol{x}_2) \;\; = \;\; \mathcal{F}^{(0)}_i(\boldsymbol{x}_1) \tag{37}$$

$$\mathcal{F}^{(1)}_{i,j}(\boldsymbol{x}_2) = r_j \mathcal{F}^{(0)}_i(\boldsymbol{x}_1) + \mathcal{F}^{(1)}_{i,j}(\boldsymbol{x}_1) \tag{38}$$

$$\mathcal{F}^{(2)}_{i,jk}(\boldsymbol{x}_2) = r^2_{jk} \mathcal{F}^{(0)}_i(\boldsymbol{x}_1) + r_j \mathcal{F}^{(1)}_{i,k}(\boldsymbol{x}_1) + r_k \mathcal{F}^{(1)}_{i,j}(\boldsymbol{x}_1) + \mathcal{F}^{(2)}_{i,jk}(\boldsymbol{x}_1), \tag{39}$$

where $\boldsymbol{r} = \boldsymbol{x}_1 - \boldsymbol{x}_2$. If the order of $\mathcal{F}(\boldsymbol{x}_1)$ and $\mathcal{F}(\boldsymbol{x}_2)$ is the same, they are equivalent; that is, $\mathcal{F}(\boldsymbol{x}_2)$ calculated by the definition and by the transformation above are identical. We denote this transformation by matrix $\mathcal{S}_F$ as

$$\mathcal{F}(\boldsymbol{x}_2) = \mathcal{S}_F(\boldsymbol{x}_2, \boldsymbol{x}_1) \cdot \mathcal{F}(\boldsymbol{x}_1). \tag{40}$$

### 3.1.3 shift-operation of velocity derivatives

Here we describe the transformation of the origin of velocity derivatives. By the definition

$$\mathcal{V}^{(m)}_{i,k\cdots}(\boldsymbol{x}_1) = \frac{1}{m!} \left[\nabla^m_{k\cdots} v_i\right](\boldsymbol{x}_1), \tag{41}$$

the velocity disturbance at $\boldsymbol{x}$ around $\boldsymbol{x}_1$ is given by

$$v_i(\boldsymbol{x}) = \sum_{m=0} \mathcal{V}^{(m)}_{i,k\cdots}(\boldsymbol{x}_1) \ (\boldsymbol{x} - \boldsymbol{x}_1)^m_{k\cdots} . \tag{42}$$

From the above equation, we get the transformation among the velocity derivatives as

$$\mathcal{V}^{(n)}_{i,l\cdots}(\boldsymbol{x}_2) = \sum_{m=n} {}_mC_n \ \mathcal{V}^{(m)}_{i,k\cdots l\cdots}(\boldsymbol{x}_1) \ (\boldsymbol{x}_2 - \boldsymbol{x}_1)^{m-n}_{k\cdots}, \tag{43}$$

or introducing the operator $\mathcal{S}_V$ as

$$\mathcal{V}(\boldsymbol{x}_2) = \mathcal{S}_V(\boldsymbol{x}_2, \boldsymbol{x}_1) \cdot \mathcal{V}(\boldsymbol{x}_1). \tag{44}$$

### 3.1.4 Procedure of FMM

In the calculation of FMM, there are mainly two stages: *upward-pass* where the force moments of the cells are calculated, and *downward-pass* where the velocity derivatives of the cells are calculated.

In the upward-pass, we calculate the force moments from particles in the cell $C$

$$\mathcal{F}(C) = \sum_{\beta \in C} \mathcal{S}_F(\boldsymbol{x}_C, \boldsymbol{x}_\beta) \cdot \mathcal{F}(\beta), \tag{45}$$

for all cells in all levels. This is achieved efficiently as follows. First, we calculate the force moment for leaves $L$ directly by the definition (45) as

$$\mathcal{F}(L) = \sum_{\beta \in L} \mathcal{S}_F(\boldsymbol{x}_L, \boldsymbol{x}_\beta) \cdot \mathcal{F}(\beta), \tag{46}$$

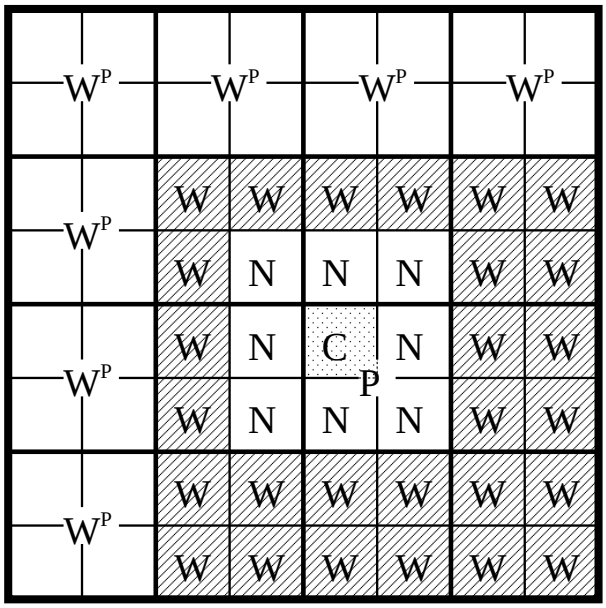


Figure 2: Cell structure in 2D. Well-separated cells of cell $C$ is denoted as $W$ and near cells of cell $C$ including itself is denoted as $N$. Well-separated cells of $C$'s parent cell $P$ is denoted as $W^P$ whose children are not $W$'s.

where $\mathcal{F}(\beta)$ is known variable for all particles $\beta$. The force moment of cell $P$ at the level $l$ is calculated by its children $C$ at the level $l-1$ by the shift operator $\mathcal{S}_F$ as

$$\mathcal{F}(P) = \sum_{C \mathrm{of} P}^{8} \mathcal{S}_F(\boldsymbol{x}_P, \boldsymbol{x}_C) \cdot \mathcal{F}(C). \tag{47}$$

By this recurrent relation, we can calculate all force moments at the levels from $l = l_m - 1$ to 2. It should be noted that the calculated values in the upward-pass is exactly the same with that by the definition (4) for the cells in principle, because the transformation of the origin of the moments (40) is exact. This gives a good check for the program.

The errors in this scheme appear at the truncation of the expansion and we have to keep a certain condition to get good estimations. For this purpose we introduce the near cells for a cell $C$ denoted by $N^C$ which does not satisfy the condition. By the near cell $N^C$, we define well-separated cells $W^C$ as follows;

- $W^C$ is at the same level of $C$.
- $W^C$'s parent is $N^P$.

- $W^C$ is not $N^C$.

By the definitions, the most important property that the well-separated cells of $C$, those of $C$'s ancestors, and the near cell of $C$ cover all region of the primary cell without overlap is satisfied. The typical definition of $N^C$ is the nearest-neighbor cells including cell $C$ itself, so that there are $3^3$ cells at most. We denote this as $n_s = 1$ where $n_s$ is the number of spacing cells to the nearest well-separated cell. Figure 2 shows that the situation in two-dimensional case for simplicity. We note that this is not the only choice but we can choose $N^C$, for example, as the cells inside the square centred by $C$ with 5 times size of $C$ ($n_s = 2$), where $5^3$ cells would be $N^C$ and the result would be more accurate.

In the downward-pass, we calculate the velocity derivatives in an efficient way. For this purpose, we introduce the velocity derivatives of the contributions from the well-separated cells of $C$ and $C$'s ancestors defined by

$$\mathcal{W}(C) = \sum_{\beta \notin N^C} \mathcal{K}(C, \beta) \cdot \mathcal{F}(\beta). \tag{48}$$

First we set zero for $\mathcal{W}$'s at level 1 (at least), because the cells at the level has no well-separated cell. By the transformation (44), we can calculate $\mathcal{W}(C)$ in terms of the parent's $\mathcal{W}(P)$ as

$$\mathcal{W}(C) = \mathcal{S}_V(\boldsymbol{x}^C, \boldsymbol{x}^P) \cdot \mathcal{W}(P) + \sum_{W^C} \mathcal{K}(C, W) \cdot \mathcal{F}(W), \tag{49}$$

where the second term in the right-hand-side is the contribution not included in $\mathcal{W}(P)$. By this relation, we can calculate $\mathcal{W}$ for all cells at the levels from $l = 2$ to $l_m$. Finally, adding the contribution from the particles in the near cells, we get the velocity derivatives for the particle $\alpha$ by

$$\mathcal{V}'(\alpha) = \mathcal{S}_V(\boldsymbol{x}^\alpha, \boldsymbol{x}^L) \cdot \mathcal{W}(L) + \sum_{\beta \in N^L, \beta \neq \alpha} \mathcal{K}(\alpha, \beta) \cdot \mathcal{F}(\beta). \tag{50}$$

### 3.1.5 Truncation

Generally errors on the multipole expansion is characterized by the order of truncation and the ratio $r/R$ where $r$ is the distance between the source and the expansion-point and $R$ is that between the observation-point and the expansion-point. In the FMM procedure, the ration $r/R$ is completely controlled by the number of spacing cell $n_s$ in the hierarchical cell-structure as

$$\frac{r}{R} \leq \frac{\sqrt{3}}{2(n_s + 1)}. \tag{51}$$

If we truncate the force moments at the order $q$ in the calculation of (48), $\mathcal{K}^{(n,m)}$ for $n + m > q$ would be negligible. We note that the expansion in § 2 is conceptually different

from the above expansion. In (25) we take into account $\mathcal{K}^{(n,m)}$ with $n, m \leq p+2$; that is, up to $\mathcal{K}^{(p+2,p+2)}$. This is because the resultant mobility problem (23) must be well-defined.

If we take larger $q$, we get more accurate $\mathcal{V}'$. However we should note that (25) with the truncation $p$ is an approximation itself. The error introduced in (25) is not clear. This is because we truncate at the same order for interactions among all particles. The truncation error would be change due to the configuration; dilute systems are more accurate than dense systems with the same truncation. The largest error in (25) would occurred on the nearest pair because $r$ is equal to $a$ and $R$ is minimized there. With $q = 2(p+2)$, the standard choice $n_s = 1$ on FMM is equivalent to the existence of pair with $R = 4/\sqrt{3} \approx 2.31$ which would be appropriate for dense systems.

### 3.1.6 Cost-estimation

Now we roughly estimate the calculation-cost on the above non-adaptive FMM scheme. Giving force moments for all particles as a trial values in the iteration, we can calculate by the following steps:

i. Assign the force moments for leaves $L$ by (46) with the cost of $O(N)$.

ii. Calculate the force moments for cells above by (47) with the cost of roughly $O(8n_C)$ where $n_C$ is the number of cells in the hierarchy.

iii. Clear $\mathcal{W}$ at level 1 with the cost of $O(1)$

iv. Calculate $\mathcal{W}$ at the levels from $l = 2$ to $l_m$ by (49) with the cost of $O\left(n_C\left(1 + n_W\right)\right)$ where $n_W$ is the number of well-separated cells for a cell.

v. Calculate the velocity derivatives of particles by (50) with the cost of $O\left(N\left(1 + n_L\right)\right)$ where $n_L$ is the number of particles in a leaf cell.

The cost of steps (ii) and (iii) are negligible for large $N$. $n_W$ is constant with $N$. $n_C$ and $n_L$ are given as

$$n_C = \sum_{l=0}^{l_m} 8^l = \frac{8^{l_m+1} - 1}{7}, \tag{52}$$

$$n_L \approx \frac{N}{8^{l_m}}, \tag{53}$$

where we expect that the configuration is homogeneous in the primary cell. If we choose $l_m \approx \log N$, it is expected that $n_C$ is $O(N)$ and $n_L$ is $O(1)$. Therefore we could calculate $\mathcal{V}'$ for all particles with the cost of $O(N)$.

After the above calculation with five steps, we return to the step (iii) on the six-step procedure in §2.4, and then we get the irreducible velocity moments $\hat{\mathcal{U}}$ corresponding to the trial force moments for the iteration method totally with the cost of $O(N)$.

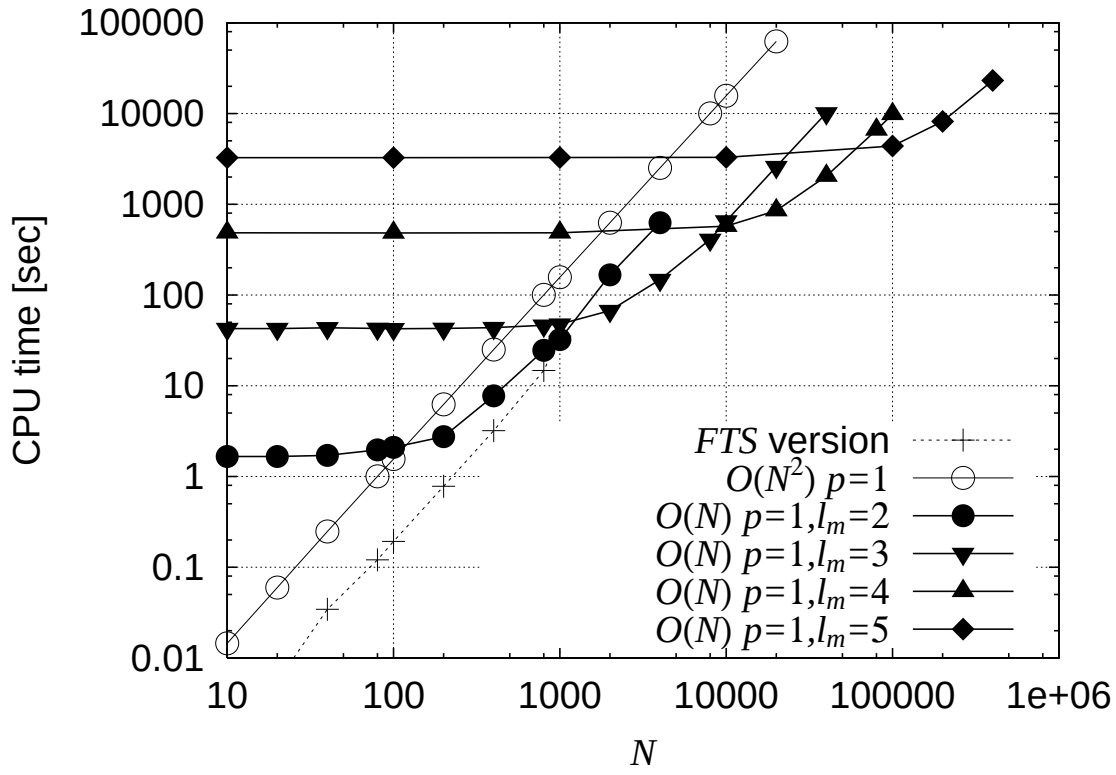


Figure 3: CPU times with the number of particles $N$. The truncation order in these calculations is $p = 1$ equivalent to $FTS$ version. The truncation order on FMM is $q = 2(p+2)$, the number of spacing cell is $n_s = 1$, and the maximum levels are $l_m = 2, 3, 4$ and 5. '$FTS$' denotes the conventional Stokedian Dynamics for comparison.

### 3.2 Results

Here we utilize the $O(N^2)$ and the $O(N)$ schemes in practice and check the performance. The calculations are done by personal computer running the FreeBSD operating system on dual Pentium III processors of 550MHz with 1GB memory. The programs are compiled by the GNU C compiler optimized for the Pentium processor.

Figure 3 shows the CPU time on the calculation of (23) with the number of particles $N$ for several calculation schemes with $p = 1$ which is equivalent to $FTS$ version. The result denoted by $O(N^2)$ uses the six-step procedure in §2.4 and the results denoted by $O(N)$ use FMM procedure on the step (ii) in the six-step procedure; that is (25). We see that the CPU time of $O(N^2)$ scheme is scaled by $N^2$ as expected. For $O(N)$ scheme with a

| $N$ | mobility | resistance |
|---|---|---|
| 4 | 5 | 8 |
| 8 | 5 | 7 |
| 10 | 9 | 53 |
| 20 | 10 | 89 |
| 40 | 9 | 105 |
| 80 | 10 | 160 |
| 100 | 11 | 211 |
| 200 | 10 | 228 |
| 400 | 10 | 327 |

Table 1: Numbers of iteration for mobility and resistance problems of the simple cubic configuration in FMM code with $p = 1$, $q = 4$, and $l_m = 2$ by BiCGSTAB2 method under the accuracy $10^{-12}$.

fixed $l_m$, we see two regions where the CPU time is almost constant with $N$ and where it is almost scaled by $N^2$. The crossover occurs where the direct particle-to-particle calculation for near cells with $O(N^2)$ cost dominates the calculation for cells with $O(N^0)$ cost for a fixed $l_m$. As suggested in §3.1.6, we need to divide the system into finer cells for larger $N$. In fact larger $l_m$ is fast for larger $N$ and the envelope line for $O(N)$ schemes is almost scaled by $N$. The result denoted by '$FTS$' is the calculation with the explicit form of the mobility matrix shown in [6, Durlofsky *et al.*(1987)]. The generalization for the truncation $p$ in $O(N^2)$ scheme makes an extra cost. For higher versions, these behaviours are also observed.

The choice of the schemes is independent from the types of the problem, because all problems – mobility, resistance, and mixed problems – consists of the irreducible generalized mobility equation (23) as the core. The total calculating cost depends on the number of iteration. Table 1 shows the number of iteration for mobility and resistance problems in FMM code. This shows that the mobility problem is solved with $O(N)$ cost, but the resistance problem need more iterations for larger $N$.

# 4 Conclusions

In this work, we have shown the formulation of the hydrodynamic interaction among rigid spherical particles in low-Reynolds-number flows with free boundary condition by the multipole expansion in real space and shown the generalized mobility problem which relates the force moments to the velocity moments. By this formulation, one of the difficulties in the conventional Stokesian Dynamics method – there is no systematic improvement on the

truncation beyond $FTS$ version – is overcome. We have also shown the improvement of the calculating speed which is the other difficulty in the Stokesian Dynamics method. First we have shown the application of iterative method to solve the linear equations appeared in the higher truncations, and have given the $O(N^2)$ scheme. Because we calculate not the velocity moments but the velocity derivatives, the fast multipole method which is a natural extension of the conventional multipole expansion can be easily applied and we have shown the non-adaptive version of the fast multipole method giving the $O(N)$ scheme with a good convergence.

By this scheme, the detailed hydrodynamic interactions for huge conglomerate of particles in a fluid which did not achieved so far due to the heavy calculations (for example, the breakup on falling in [17] and by shear in [12]) are tractable. Not only for this type of direct application, the formulation would be easily applicable for other problems such as liquid-liquid systems and for periodic boundary condition, due to the simple formulation. The adaptive version of the fast multipole method does not discussed in this work, but this would be important for the practical studies, because we usually meet the structures or the patterns.in the systems and the non-adaptive version hardly handles the situations.

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