

NUMERICAL DETERMINATION OF TRUNCATION ORDERS IN THE CORRECTION METHOD FOR STOKES EQUATIONS

Minh-Phuong TRAN ^{1,*}, Thanh-Nhan NGUYEN ²

¹Faculty of Mathematics - Statistics, Ton Duc Thang University,
Ho Chi Minh City, Vietnam

²Department of Mathematics, Ho Chi Minh City University of Education,
Ho Chi Minh City, Vietnam

*Corresponding Author: Minh Phuong TRAN (email: tranminhphuong@tdt.edu.vn)
(Received: 07-December-2017; accepted: 07-February-2018; published: 31-March-2018)

DOI: <http://dx.doi.org/10.25073/jaec.201821.85>

Abstract. In [15], the authors propose an accurate method, namely the correction method, for computing hydrodynamic interaction between very closed spherical particles in a Stokes fluid. The accuracy of this method depends on two truncation parameters for approximating the Neumann to Dirichlet matrix and the velocity correction respectively. In this paper, we establish a numerical determination to estimate these parameters. We perform some numerical experiments to present our method.

Key Words: Stokesian Dynamics, Stokes equation, Hydrodynamic interaction, Truncation order.

1. Introduction

In recent papers, many mathematicians have studied the hydro dynamic interactions between close particles immersed in a Stokes fluid to simulate the motions of nano scale swimmers robots which is designed from nano-sized medical devices (see [2], [3] and references therein). One of the main difficulties is to compute the total forces and torques exerted by the particles. Our work is motivated by this problem.

We consider N non intersecting particles immersed in a viscous fluid. For simplicity, the particles are identical balls B_1, B_2, \dots, B_N with radius 1 and centers $z_1, z_2, \dots, z_N \in \mathbb{R}^3$, respectively. We assume that the closed balls B_i do not intersect and that the fluid fills the rest of the space. The fluid occupies the domain $\Omega := \mathbb{R}^3 \setminus \left(\bigcup_{i=1}^N B_i\right)$. We assume moreover that the fluid inertia effects are negligible compared to the viscosity (i.e. the Reynolds number is very small $Re \ll 1$) so that the velocity u and the pressure p solve the stationary Stokes equations in the fluid domain,

$$\nabla \cdot \sigma = 0, \quad \nabla \cdot u = 0 \quad \text{in } \Omega, \quad (1)$$

where $\sigma = \nabla u + \nabla u^T - p\text{Id}$ is the stress tensor in the fluid and Id is the identity matrix. On the surfaces of the particles, we consider a no-slip boundary condition,

$$u = u_i \quad \text{on } \partial B_i, \quad i = 1, 2, \dots, N.$$

where the velocity u_i corresponds to a rigid displacement. It is characterized by the velocity \mathbf{U}_i at the center z_i of the ball B_i and by the angular velocity ω_i ($\mathbf{U}_i, \omega_i \in \mathbb{R}^3$),

$$u_i(x) := \mathbf{U}_i + \omega_i \times (x - z_i), \quad \text{for } x \in \mathbb{R}^3. \quad (2)$$

We are interested in solutions which decay at infinity, i.e., which fulfills $u(x) \rightarrow 0, p(x) \rightarrow$

0, as $|x| \rightarrow \infty$. The existence and uniqueness of a solution to (1) is classical in the Hilbert space (see [10] and [17]).

The surface density of force exerted on the fluid at some point x of the surface ∂B_i is given by

$$f_i(x) = (\nabla u + \nabla u^T - p\text{Id}) \cdot n_i, \quad (3)$$

where n_i denotes the exterior normal on the surface of the particle B_i . The total force and total torque exerted by the particle B_i on the fluid are given by the following formulas,

$$F_i = \int_{\partial B_i} f_i(x) dS(x),$$

$$T_i = \int_{\partial B_i} (x - z_i) \times f_i(x) dS(x).$$

We recall that the solution to the transmission problem u is given by the convolution of the surface force density f_i with the Green tensor for the Stokes equation as follows

$$u(x) = \sum_{i=1}^N \int_{\partial B_i} G(x-y) f_i(y) dS(y), x \in \mathbb{R}^3 \quad (4)$$

This explicit formula gives the velocity field everywhere as soon as the force densities f_i are known. However, the data of the problem are the velocity field u_i , not these force densities. We are led to consider the following ‘‘Dirichlet to Neumann operator’’

$$DN : (u_{|\partial B_1}, \dots, u_{|\partial B_N}) \longmapsto (f_1, \dots, f_N).$$

This operator is positive and symmetric, its inverse is the corresponding ‘‘Neumann to Dirichlet operator’’ ND . In the initial problem, we only need to compute approximations of DN when $(u_{|\partial B_i})_{1 \leq i \leq N}$ is a finite sequence of rigid motion. Moreover, we do not need a complete description of $(f_i)_{1 \leq i \leq N}$ but only the projections of these densities. In short, we only need a projection of the operator DN on a finite dimensional space of dimensions $6N$. This projection is called the friction operator as follows

$$\mathcal{F} : \mathbb{R}^{6N} \longrightarrow \mathbb{R}^{6N},$$

$$(U_i, \omega_i)_{1 \leq i \leq N} \longmapsto (F_i, T_i)_{1 \leq i \leq N}.$$

Unfortunately, we do not have a nice explicit expression for DN such as (4). To compute accurate approximations of \mathcal{F} starting from (4),

the direct method consists in 1/ approximating ND by a Galerkin method, 2/ inverse this approximate operator, 3/ project this inverse on the space of rigid motions. For a fixed position of the particles, the direct method has a very good behavior as we send the truncating order to infinity. On the contrary, if we consider a sequence of configurations with at least two particles getting closer and closer and with different prescribed velocities, the distributions of forces concentrate near the contact points. In this case, the convergence of the direct method degenerates.

A large amount of research has been studied to develop numerical tools to approximate the friction operator, such as [5], [6], [8], [9], [13]. Recently, in [15], the authors developed a method which is called the correction method for computing very accurate numerical solutions. This method depends on two truncating parameters for approximating the Dirichlet to Neumann operator DN and computing the correction velocities respectively. In the correction method, these parameters are chosen to obtain a good approximation of friction operator. The main goal of this paper is to present a numerical method to determine truncating parameters for the correction method.

The rest of this paper is organized as follows. In the next section, we describe the main idea of the correction method which is based on the singular-regular decomposition. We also present the interpolation method for computing the singular fields and the computation of correction velocities for two close particles. In Section 3. , we propose some numerical computations to estimate the truncation orders using in the correction method. In Section 4. , numerical experiments are performed for four particles problem. Finally, we give several conclusions and perspectives in the last section.

2. The correction method

2.1. Singular-regular splitting

Let us first introduce a cut-off distance $\delta > 0$. We denote by d_{ij} the distance between two par-

ticles B_i and B_j , $d_{ij} = |z_i - z_j| - 2$. The set of pairs of close particles is defined as

$$\mathcal{P} = \{(i, j) \in \{1, \dots, N\}^2, i \neq j : d_{ij} < \delta\}.$$

Our method consists in taking advantage of the linearity of the Stokes equations for rewriting the fields (u, p) as a superposition

$$u = u^0 + \sum_{c \in \mathcal{P}} u^c, \quad p = p^0 + \sum_{c \in \mathcal{P}} p^c,$$

where each couple (u^0, p^0) solves the Stokes equations in Ω and (u^c, p^c) solves the Stokes equations in the fictitious fluid domain:

$$\Omega^c = \mathbb{R}^3 \setminus \{B_i \cup B_j\}, \quad \text{for } c = (i, j) \in \mathcal{P}.$$

The couple (u^c, p^c) handle the large variations of (u, p) localized in the small gap between B_i and B_j which are due to the difference between the prescribed velocities on ∂B_i and ∂B_j . Precisely, for $c = (i, j) \in \mathcal{P}$, we introduce the velocity field

$$w^c(x) := \frac{1}{2}[u_j(x) - u_i(x)],$$

which vanishes if and only if the solid $B_i \cup B_j$ follows a rigid motion. The “singular” field (u^c, p^c) are defined as the unique solution of the problem

$$\begin{cases} -\Delta u^c + \nabla p^c = 0 & \text{in } \Omega^c, \\ \nabla \cdot u^c = 0 & \text{in } \Omega^c, \\ u^c = -w^c & \text{on } \partial B_i, \\ u^c = w^c & \text{on } \partial B_j, \\ u^c(x) \rightarrow 0, p^c(x) \rightarrow 0 & \text{as } |x| \rightarrow \infty. \end{cases} \quad (5)$$

By linearity, the remaining part (u^0, p^0) solves the Stokes problem in Ω . The boundary conditions u^0 for this problem are set so that the total velocity field satisfies the boundary conditions u_i specified in the original problem

$$\begin{cases} -\Delta u^0 + \nabla p^0 = 0 & \text{in } \Omega, \\ \nabla \cdot u^0 = 0 & \text{in } \Omega, \\ u^0 = w^0 & \text{on } \partial B_i, \\ u^0(x) \rightarrow 0, p^0(x) \rightarrow 0 & \text{as } |x| \rightarrow \infty, \end{cases} \quad (6)$$

where,

$$w^0(x) := u_i(x) - \sum_{c \in \mathcal{P}} u^c(x), \quad x \in \partial B_i. \quad (7)$$

At the end we aggregate the different contributions. With obvious notation, for $k = 1, 2, \dots, N$,

$$F_k = F_k^0 + \sum_{c \in \mathcal{P}} F_k^c, \quad T_k = T_k^0 + \sum_{c \in \mathcal{P}} T_k^c.$$

Notice that the singular solution (u^c, p^c) associated to a pair of close particles $c = (i, j) \in \mathcal{P}$ do not contribute to the forces and torques exerted by the surface of a third particle B_k , $k \notin \{i, j\}$: we have $F_k^c = T_k^c = 0$. Indeed, in this case, $B_k \subset \Omega^c$, so that by the Stokes formula,

$$F_k^c = \int_{\partial B_k} \sigma^c(x) \cdot n_k(x) dS = \int_{B_k} \nabla \cdot \sigma^c(x) dx = 0.$$

Similarly, using the Levi-Civita antisymmetric symbol $\varepsilon_{\alpha\beta\gamma}$ and Einstein summation convention on greek indices, we compute,

$$\begin{aligned} T_k^c &= \int_{\partial B_k} n_k(x) \times (\sigma^c \cdot n_k(x)) dS \\ &= \varepsilon_{\alpha\beta\gamma} \int_{\partial B_k} n_\beta \sigma_{\gamma\zeta}^c n_\zeta dS \\ &= \varepsilon_{\alpha\beta\gamma} \int_{B_k} \frac{\partial}{\partial x_\zeta} [(x - z_i)_\beta \sigma_{\gamma\zeta}^c] dx \\ &= \varepsilon_{\alpha\beta\gamma} \int_{B_k} (x - z_i)_\beta \underbrace{(\nabla \cdot \sigma^c)_\gamma}_{=0} dx \\ &\quad + \int_{B_k} \underbrace{\varepsilon_{\alpha\beta\gamma} \sigma_{\gamma\beta}^c}_{=0} dx = 0. \end{aligned}$$

As a consequence, the total force and torque exerted by the particle B_k on the fluid are given by

$$\begin{aligned} F_k &= F_k^0 + \sum_{\substack{c=(i,j) \in \mathcal{P}, \\ k \in \{i,j\}}} F_k^c, \\ T_k &= T_k^0 + \sum_{\substack{c=(i,j) \in \mathcal{P}, \\ k \in \{i,j\}}} T_k^c. \end{aligned} \quad (8)$$

The advantage of decomposing the solution resides in the possibility of using different methods for solving problems (5) and (6). The singular parts are solution of the Stokes equations (5) around only two solid particles. We will approximate these singular parts by interpolating in pre-computed tables. The remaining parts solves the Stokes equations (6) in the original domain but with modified boundary conditions

which do not necessarily correspond to rigid motions of the particles. The remaining regular part may be approximated by using any standard numerical method.

Let us first consider problem (5). For $c = (i, j) \in \mathcal{P}$, by changing coordinates, we may assume that $z_i = -(1 + d_c/2)e_z$ and $z_j = (1 + d_c/2)e_z$. In the new coordinates, the velocity w^c uniquely decomposes as

$$w^c(x) = U_z^c e_z + U_{xy}^c e_1 + \omega_z^c e_z \times x + \omega_{xy}^c e_2 \times x,$$

where e_1 and e_2 are two unit vectors orthogonal to e_z . Hence, the solution of (5) can be decomposed as

$$(u^c, p^c) = U_z^c(u_A, p_A) + U_{xy}^c(u_B, p_B) + \omega_{xy}^c(u_{B'}, p_{B'}) + \omega_z^c(u_C, p_C), \quad (9)$$

where, for $Z = A, B, B'$, or C , the couple (u_Z, p_Z) solves the Stokes equations in the domain

$$\Omega^{d_c} := \mathbb{R}^3 \setminus [B_+^{d_c} \cup B_-^{d_c}], \quad (10)$$

where $B_\pm^{d_c}$ denotes the solid sphere with unit radius and center $\pm(1 + d_c/2)e_z$. The difference between these problems comes from the specific boundary conditions,

$$u_Z = w_Z \quad \text{on } \partial B_+^{d_c} \cup \partial B_-^{d_c},$$

where w_Z are defined as follows, for $x \in \partial B_\pm^{d_c}$,

$$\begin{aligned} w_A(x) &:= \pm e_z, \quad w_B(x) := \pm e_1, \\ w_{B'}(x) &:= \pm e_2 \times x, \quad w_C(x) := \pm e_z \times x. \end{aligned} \quad (11)$$

When solving independently the second or the third problem, we may rotate the frame so that e_1 or e_2 coincide with e_x . We end with four family of problems only depending on the distance d_c . More precisely, in view of (8), we need approximations of

$$F_Z(d_c) := \int_{\partial B_+^{d_c}} \sigma_Z(x) \cdot n(x) dS(x), \quad (12)$$

$$T_Z(d_c) := \int_{\partial B_+^{d_c}} n(x) \times [\sigma_Z(x) \cdot n(x)] dS(x). \quad (13)$$

Using the symmetries of the problems, the corresponding total forces and torques on $\partial B_-^{d_c}$ are

deduced from the former. For the computation of the boundary conditions (7) satisfied by the remaining ‘‘regular part’’ (u^0, p^0) , we also need approximations of $v_Z(x, d_c) := u_Z(x)$, for $x \in \Omega^{d_c}$ and $Z = A, B, B', C$.

In the next section, we describe a procedure for computing these quantities. The method is based on known asymptotic as $d_c \rightarrow 0$, direct computations and interpolation in the parameter d_c .

Let us now consider problem (6). It is of the same nature as the original problem: solve the Stokes equations in the fluid domain surrounding the particles. The new problem looks even more complex since we have substituted the function w^0 for the simple rigid motions u_i that can be described with $6N$ parameters. However, by construction, (u^0, p^0) is a very regular vector field, even in the limit of touching particles. As a consequence, applying standard numerical methods to problem (6), we can compute approximations of (u^0, p^0) with an accuracy that does not depend on the distance d_c between close particles.

In the next section, we describe a procedure for computing the approximations of the singular part and the boundary condition for the regular part. The main idea is to interpolate the needed quantities into a grid of known values which has been computed once for all during a pre-processing step.

2.2. The interpolation method for computing the singular fields

As explained in the discussions at the end of Section 2.1., for each $c = (i, j) \in \mathcal{P}$, the singular part (u^c, p^c) can be decomposed as a combination of four parts (u_Z, p_Z) which are solutions of four family of problems only depending on the distance d_c ,

$$\begin{cases} -\Delta u_Z + \nabla p_Z = 0 & \text{in } \Omega^{d_c}, \\ \nabla \cdot u_Z = 0 & \text{in } \Omega^{d_c}, \\ u_Z = w_Z & \text{on } \partial \Omega^{d_c}, \end{cases} \quad (14)$$

where Ω^{d_c} and w_Z are given by (10) and (11) respectively. Recall that the fluid domain Ω^{d_c} only

depends on the distance d_c . We need to compute direct approximations of f_Z and T_Z given by (12), (13). Our method is based on asymptotic formulas for the total force and torque at small distance, direct computations and interpolation in the parameter d_c .

In a pre-processing step, we decompose $(\tilde{f}_Z)_k$ and $(w_Z)_k$, for $k = B_-^{d_c}, B_+^{d_c}$, in the basis of vector spherical harmonics (see [16]) as follows,

$$(\tilde{f}_Z)_k = \sum_{\alpha \geq 0} f_{k,\alpha}^Z \phi_{k,\alpha}, \quad (w_Z)_k = \sum_{\alpha \geq 0} w_{k,\alpha}^Z \phi_{k,\alpha}.$$

By truncating the above series up to order M_{max} , with M_{max} large, the discrete Neumann to Dirichlet matrix $\mathcal{N}\mathcal{D}_{Z,dis}$ is computed as described in [18]. Then we compute accurate approximations of the surface force density f_Z^{dis} by solving the linear problem,

$$ND_{Z,dis} \cdot f_Z^{dis} = W_Z,$$

where $W_Z = (w_{i,\alpha}^Z)_{k=i,j,\alpha=1,\dots,M_{max}}$. By this direct method, we may compute f_Z^{dis} as a function of d_c for a finite number of distances, say $d_c \in \mathcal{D}^{dis} := \{d_0, \lambda d_0, \lambda^2 d_0, \dots\}$ for some small d_0 and some $\lambda > 1$. Combining the explicit asymptotic formula of the force density with this discrete set of accurately computed values, we obtain approximations of $f_Z^{dis}(d_c)$ by interpolation for every $0 < d_c < \delta$.

For instance, let us consider the first problem $Z = A$. We are interested in the total force and torque exerted by the first particles $B_-^{d_c}$. In this case, from the symmetries and the asymptotic formulas given by (see [7])

$$F^A(d_c) = \left(\frac{3\pi}{d_c} + O(\ln d_c) \right) e_z, \quad T_A(d_c) = 0,$$

We guess that $F^A(d_c)$ expands as

$$F^A(d_c) = \left[\frac{3\pi}{d_c} + C_1 \ln d_c + C_2 + C_3(d_c \ln d_c) + C_4 d_c + \mathcal{R}_A(d_c) \right] e_z.$$

The constants C_1, C_2, C_3 and C_4 are then determined by using a least square approximation based on highly accurate numerical simulations performed for a small number of small values of

d_c . The Figure 1 shows the behavior of the rest term $\mathcal{R}_A(d_c)$.

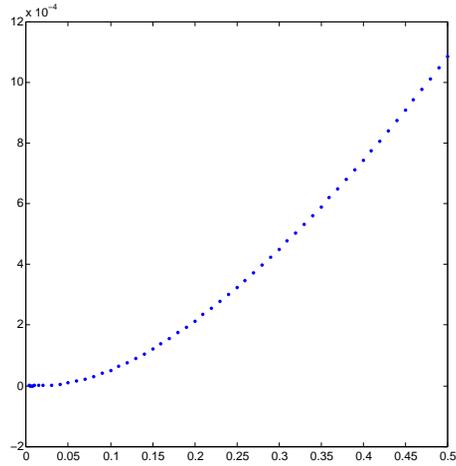


Fig. 1: The term $\mathcal{R}_A(d_c)$ in a function of d_c .

Tab. 1: The absolute errors of interpolation.

d_c	0.475	0.355	0.275	0.135	0.0135
L_{max}	50	50	50	70	150
error	4.4e-13	2.2e-12	3.5e-12	7.4e-12	3.1e-10

In a second step we build a table of values of $\mathcal{R}_A(d_c)$ for d_c ranging in a finite subset of $(0, \delta)$. These values are obtained by the direct method with a very large L_{max} .

In practice, we have performed accurate simulations with the following distances:

$$d_c = 0.001, 0.002, \dots, 0.009, 0.01, 0.02, \dots, 0.5.$$

This ends the preprocessing step.

Eventually, when needed, we use the cubic spline interpolation method to estimate $\mathcal{R}_A(d_c)$ for any non-tabulated distance $d_c \in (0, \delta)$ from the tabulated values. In Table 1, we show the result of some numerical tests realized in order to estimate the error due to the interpolation method.

2.3. Computation of correction velocities

In this section, we present the interpolation method to compute the coefficients of the correction velocities.

We consider again the problem (14). Let B_R be the ball of radius $R = 3$ centered at the origin of the coordinate system. This ball contains the two balls $B_-^{d_c}$ and $B_+^{d_c}$. We want to determine the velocity $\mathbf{U}_Z(r, d_c)$ for $r \in \mathbb{R}^3 \setminus B_R$.

We first compute the force densities on the boundary of $B_+^{d_c}$ and $B_-^{d_c}$ using the direct method with a large truncating order. Then, we can deduce the velocity field \mathbf{U}_Z everywhere using the explicit formula (4) and vector spherical harmonics (see [18]). On the other hand, we know that the velocity field in $\mathbb{R}^3 \setminus B_R$ reads

$$\begin{aligned} \mathbf{U}_Z(r, d_c) = & \sum_{l \geq 1} \sum_{|m| \leq l} g_{Z,l,m}^T(d_c) |r|^{-(l+1)} T_{l,m} \\ & + \sum_{l \geq 0} \sum_{|m| \leq l+1} g_{Z,l,m}^I(d_c) |r|^{-(l+1)} I_{l,m} \\ & + \sum_{l \geq 1} \sum_{|m| \leq l-1} \left[\frac{(2l-3)(l-1)}{2l} g_{Z,l-2,m}^I(d_c) (|r|^2 - 1) \right. \\ & \left. + g_{Z,l,m}^N(d_c) \right] |r|^{-(l+1)} N_{l,m}, \end{aligned} \quad (15)$$

We then only have to tabulate the coefficients $g_{Z,l,m}^T, g_{Z,l,m}^I, g_{Z,l,m}^N$. These coefficients are obtained by projecting $\mathbf{U}_Z(\cdot, d_c)$ on the basis of rescaled vector spherical harmonics on ∂B_R . In a last step, we use (15) to obtain the corresponding coefficients in the vector spherical harmonic basis on $\partial B(0, 1)$.

In practice, the series (15) is truncated at some order \tilde{L}_{max} . We call \tilde{L}_{max} the correction truncation order. Notice that this truncation order may be different than L_{max} defined in [18]. The choice of \tilde{L}_{max} will be discussed in the next section.

Finally, using a polynomial interpolation of these computed coefficients, we can estimate the coefficients of the correction velocities on the unit sphere for any $d_c \in \mathcal{D}^{dis}$.

These coefficients are computed as functions of the distance d_c in the four cases corresponding to $Z = A, B, B', C$. As an example, we show the absolute error of the polynomial interpolation corresponding to one coefficient in Figure 2.

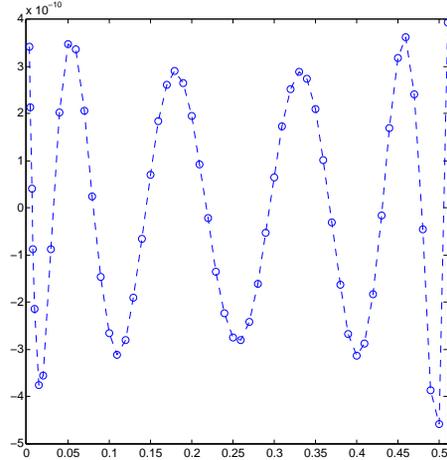


Fig. 2: The absolute errors of interpolation correspond to the coefficient $g_{Z,5,0}^N(d_c)$ (right) in function of d_c in the case $Z = A$.

3. Numerical determination of the truncation orders

In the correction method, when we approximate the correction w^0 determined by (7) and the Neumann to Dirichlet matrix \mathcal{DN} , we have to choose two truncating parameters: L_{max} for approximating the Neumann to Dirichlet matrix and \tilde{L}_{max} for approximating the velocity corrections. These quantities prescribe the number of vector spherical harmonics used for the discretization. The natural question is how can we choose these parameters such that the solution has a given accuracy? How do they depend on the distances between the particles? In this section, we present a numerical estimation of these parameters.

3.1. Correction truncation order

Let us consider the problem (1) with three unit balls. We assume that their centers lie on the vertical axis with corresponding coordinates $z_1 = (0, 0, 0)$, $z_2 = (0, 0, 2 + d)$, and $z_3 = (0, 0, 4 + d + D)$. We assume moreover that the two first balls translate along the vertical axis with opposite velocities and that the third

particle moves with the same velocity of the second one, i.e., the given velocities of three balls are respectively $u_1 = -e_z$ and $u_2 = u_3 = e_z$.

Firstly, we write the surface densities as functions of the distances between the particles and of the truncating parameters

$$f^{dis.}(L, \tilde{L}) = f^{dis.}(d, D, L, \tilde{L}),$$

where L and \tilde{L} are respectively the truncation orders used for approximating the Neumann to Dirichlet matrix and for the velocity corrections.

Since the correction method converges very fast, we may fix a large enough value of the truncation order $L = L_0$ for estimating \tilde{L}_{max} . In numerical tests we choose $L_0 = 20$. Then for every $\tilde{L} \in [1, \tilde{L}_\infty)$, we define the error for the surface density as follows

$$Err := \left| f^{dis.}(L_0, \tilde{L}) - f^{dis.}(L_0, \tilde{L}_\infty) \right|,$$

where \tilde{L}_∞ is very large.

Given a real small number $\varepsilon > 0$, the truncation order \tilde{L}_{max} is chosen as follows

$$\tilde{L}_{max}(d, D) := \min \left\{ \tilde{L} \in [1, \tilde{L}_\infty) : Err < \varepsilon \right\}.$$

In our numerical experiments, we set $\varepsilon = 10^{-6}$. Moreover, we only consider $d < \delta$, where $\delta = 2$ is the cut-off distance defined in Section 2.1. Then we numerically calculate $\tilde{L}_{max}(d, D)$ as a function of d and D (see Figure 3).

Figure 3 shows that the truncation order \tilde{L}_{max} for computing the velocity correction mainly depends on D . This truncation order can be used to estimate the other truncation order L_{max} in the next section.

Here we perform the tests with D vary from 0.1 to 5. We can choose

$$\tilde{L}_{max}(D) = \begin{cases} 10 & \text{for } D \geq 3, \\ 12 & \text{for } 2 \leq D < 3, \\ 14 & \text{for } 1.5 \leq D < 2, \\ 16 & \text{for } 0.7 \leq D < 1.5, \\ 18 & \text{for } 0.6 \leq D < 0.7, \\ 22 & \text{for } 0.3 \leq D < 0.6, \\ 24 & \text{for } 0.1 \leq D < 0.3. \end{cases}$$

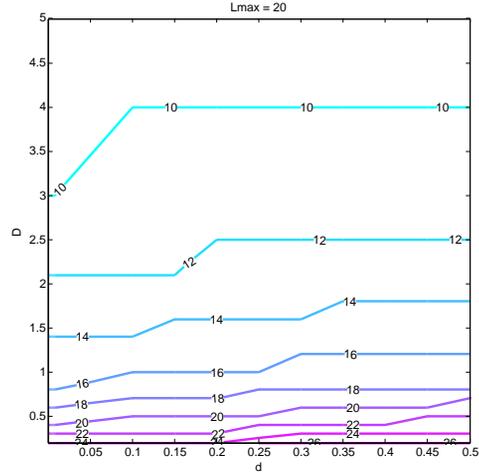


Fig. 3: Estimations of $\tilde{L}_{max}(d, D)$.

3.2. Truncation order for solving the problem

We now consider the same three-sphere configuration as in the previous section. For computational time problem, we could not calculate $f^{dis.}(L, \tilde{L}_{max})$ for very large values of L . The error on the surface force density is estimated by the difference between two consecutive values of L with \tilde{L}_{max} determined in the previous section. For every $L \geq 1$, we define

$$Err := \left| f^{dis.}(L, \tilde{L}_{max}) - f^{dis.}(L-1, \tilde{L}_{max}) \right|, \tag{16}$$

The truncation order L_{max} is chosen as follows, for a given small real number $\varepsilon > 0$,

$$L_{max}(d, D) := \min \{ L \in [1, \infty) : Err < \varepsilon \}.$$

In fact, the truncation order L_{max} can be also estimated with another definition of the density error,

$$\widetilde{Err} = \left| f^{dis.}(L, \tilde{L}_\infty) - f^{dis.}(L-1, \tilde{L}_\infty) \right|,$$

where \tilde{L}_∞ is very large. The two errors are very close in the numerical computation. Hence, it is more convenient to use the first definition (16).

We also choose $\varepsilon = 10^{-6}$ and the cut-off distance $\delta = 2$. We consider two cases: $D > \delta$ and $D < \delta$.

- The first case: $D = D_0 > \delta$,

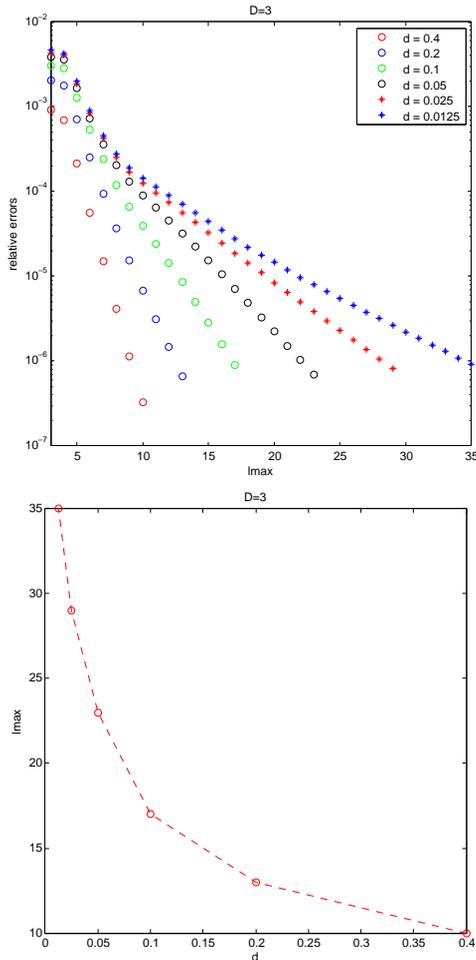


Fig. 4: First: the error $Err(d, D_0, L)$ with $D_0 > \delta$. Second: the corresponding $L_{max}(d, D_0)$ as a function of d .

In this case, the truncation order mainly depends on the distance d . We conclude that for isolated pairs of particles $D \geq \delta$, we see that the critical truncation level is a monotonic increasing function of d .

We can choose

$$L_{max}(d) = \begin{cases} 10 & \text{for } d \geq 0.5, \\ 11 & \text{for } 0.2 \leq d < 0.5, \\ 12 & \text{for } 0.18 \leq d < 0.2, \\ 13 & \text{for } 0.15 \leq d < 0.18, \\ 14 & \text{for } 0.1 \leq d < 0.15, \\ 15 & \text{for } 0.01 \leq d < 0.1. \end{cases}$$

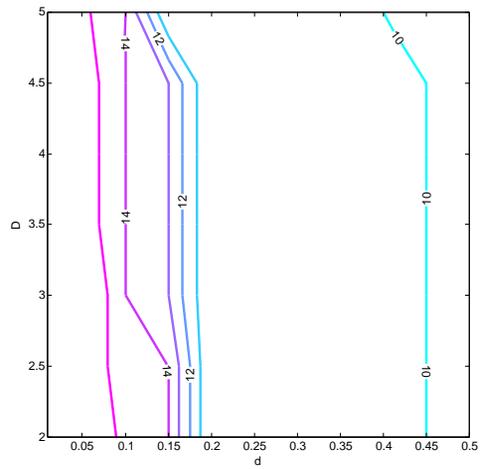


Fig. 5: Estimations of $L_{max}(d, D)$ for $D \geq \delta = 2$.

We made these tests with d varying from 0.01 to 0.5. Even for $d = 0.01$, the truncation order $L_{max} = 15$ lead to an error smaller than $\varepsilon = 10^{-6}$ (see Figure 5).

- The second case: $D = D_0 < \delta$,

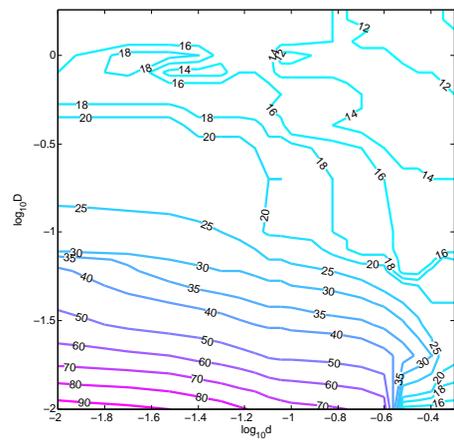


Fig. 6: $L_{max}(d, D)$ for $D \leq \delta = 2$.

In this case, the optimal truncation order depends on both d and D . This truncation order tends to infinity as both d and D go to 0.

In practice, we see on the graphic that we can choose L_{max} as an affine function of $\log_{10} D$ and $\log_{10} d$ in the region of $[L_{max, opt} \geq 40]$ (see Figure 6).

4. Numerical results

In this section, we perform some numerical tests to compare the three methods: the direct method in [11], the Stokesian Dynamics in [5] and the correction method. Recall that in the case of two particles, the correction method and the Stokesian Dynamics are exactly the same. Hence we just consider the cases with more than two particles.

We consider four particles such that their centers are not on a straight line. These centers are respectively

$$z_1 = 0, \quad z_2 = (2 + d)e_a, \\ z_3 = z_2 + (2 + d)e_b, \quad z_4 = z_3 + (2 + d)e_c,$$

where $d = 0.05$ is the distance of particles and e_a, e_b, e_c are unit vectors as follows

$$e_a = \left(\frac{1}{\sqrt{3}}, \frac{1}{\sqrt{3}}, \frac{1}{\sqrt{3}} \right), \\ e_b = \left(\frac{1}{\sqrt{4}}, \frac{1}{\sqrt{5}}, \sqrt{\frac{11}{20}} \right), \\ e_c = \left(\frac{1}{\sqrt{2}}, \frac{1}{\sqrt{6}}, \frac{1}{\sqrt{3}} \right).$$

The rigid displacements u_i are given by (2), where the corresponding velocities \mathbf{U}_i and angular velocities ω_i are given by

$$\mathbf{U}_1 = (1, -2, 3), \quad \mathbf{U}_2 = (-2, 3, 0), \\ \mathbf{U}_3 = (3, 0, -1), \quad \mathbf{U}_4 = (-1, -1, 1), \\ \omega_1 = (2, 0, -3), \quad \omega_2 = (-1, -2, 0), \\ \omega_3 = (2, 1, -2), \quad \omega_4 = (-1, -1, 1).$$

We show the numerical results in two steps: first we compare the three methods in Figure 7 and then we compare the two best methods in Figure 8. The behavior of the total forces and torques on four particles are slightly the same in three directions. So we show below the force on the particle B_2 in z direction.

Zooming on the results of the Stokesian Dynamics and the correction method (see Figure 8), we see that the latter has a better behavior. With $L_{max} = 8$, the relative error for the correction is smaller than 6.10^{-6} . So we conclude that even in the presence of several parti-

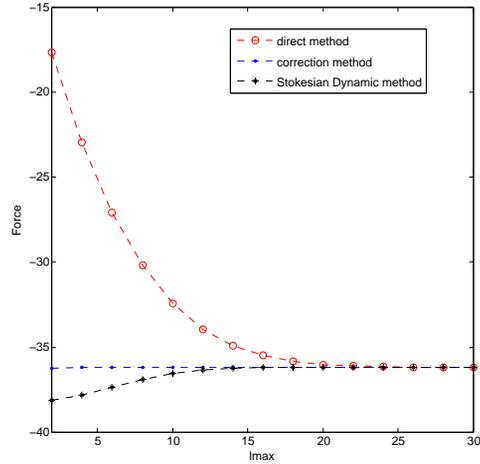


Fig. 7: Forces on the particle B_2 in z direction computed with the three methods with $d = 0.05$.

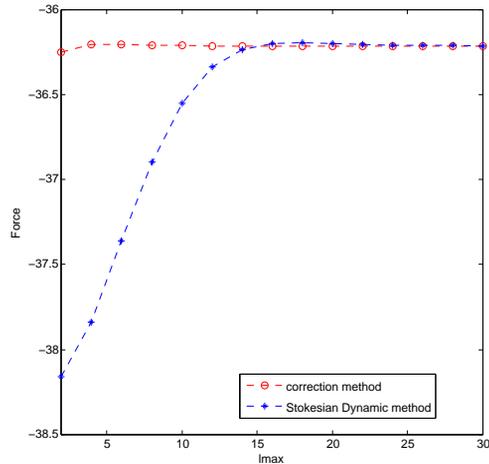


Fig. 8: Forces on the particle B_2 in z direction computed with the Stokesian Dynamics and the correction method: B_1 (first), B_2 (second), B_3 (third) and B_4 (fourth). $d = 0.05$.

cles the correction method also improves the approximation of the interactions with neighboring particles.

Let us state again the main difference between these methods. The Stokesian Dynamics modifies the interaction of each pair of close particles independently. The correction method also modifies the interactions with neighboring particles. Hence at the same level of truncation order, the computational time of the correction method is larger. But the correction method converges

very fast and requires a small level of truncation order to get an accurate result.

5. Conclusions and perspectives

In conclusion, we have presented an accurate method for the computations of hydrodynamic forces between spherical particles suspended in a Stokes fluid. The main improvement of this new method compared with the Stokesian Dynamics is that the influence of the singular force densities between two closed particles on the neighboring particles is also computed. For this reason, the computational cost for this method is larger. The main part of the computational time is due to the computation of the correction velocities and their projection on the vector spherical harmonics basis. On the other hand, these computations are independent from one sphere to another and could be easily parallelized. This should solve the main drawback of the method. Moreover, we proposed some numerical determination for some parameters using in this method.

In our research, we only consider spherical particles. The main advantage of this shape is that the computation can be based on the vector spherical harmonics basis. The methods generalize to arbitrary smooth particles. In this case, we should use a boundary finite element method instead of the decomposition in vector spherical harmonics.

Acknowledgment

The second author was supported by Ho Chi Minh City University of Education, grant CS2016.19.17.

References

- [1] AGMON, S., A. DOUGLIS, L. NIRENBERG, "Estimates near the boundary for solutions of elliptic partial differential equations satisfying general boundary conditions", *Comm. Pure Appl. Math.*, vol. 12, pp. 623-727, 1959.
- [2] ALOUGES, F., A. DESIMONE, L. HELTAI, A. LEFEBVRE, B. MERLET, "Optimally swimming stokesian robots," *Discrete Contin. Dyn. Syst. Ser. B*, vol. 18, no. 5, pp. 1189-1215, 2013.
- [3] ALOUGES, F., A. DESIMONE, A. LEFEBVRE, "Optimal strokes for low Reynolds number swimmers: an example," *J. Nonlinear Sci.*, vol. 18, no. 3 pp. 277-302, 2008.
- [4] BOSSIS, G., J.-F. BRADY, "Dynamic simulation of sheared suspensions. I. General method," *J. Chem. Phys.*, vol. 80, no. 10, pp. 5141-5154, 1984.
- [5] BRADY, J.-F., G. BOSSIS, "Stokesian dynamics," *Ann. Rev. Fluid Mech.*, vol. 20, pp. 57-111, 1988.
- [6] CICHOCKI, B., B.-U. FELDERHOF, K. HINSEN, E. WAJNRYB, J. BLAWZDZIEWICZ, "Friction and mobility of many spheres in stokes flow," *J. Chem. Phys.*, vol. 100, pp. 3780, 1994.
- [7] COX, R.-G., "The motion of suspended particles almost in contact," *Int. J. Multiphase Flow*, vol. 1, no. 2, pp. 343-371, 1974.
- [8] DURLOFSKY, L.-J., J.-F. BRADY, "Dynamic simulation of bounded suspensions of hydrodynamically interacting particles," *J. Fluid Mech.*, vol. 200, pp. 39-67, 1989.
- [9] DURLOFSKY, L.-J., J.-F. BRADY, G. BOSSIS, "Dynamic simulation of hydrodynamically interacting particles," *J. Fluid Mech.*, vol. 180, pp. 21-49, 1987.
- [10] GALDI, G.-P., *An introduction to the mathematical theory of the Navier-Stokes equations. Vol. I.* Springer-Verlag, 1994, New York. ISBN 0-387-94172-X.
- [11] HALPERN, L., "A spectral method for the Stokes problem in three-dimensional unbounded domains," *Math. Comp.*, vol. 70, no. 236, pp. 1417-1436 (electronic), 2001.

- [12] HANNAY, J.-H., J.-F. NYE, "Fibonacci numerical integration on a sphere," *J. Phys. A*, vol. 37, no. 48, pp. 11591–11601, 2004.
- [13] LADD, A.-J. C, " Hydrodynamic interactions in a suspension of spherical particles," *J. Chem. Phys.*, vol. 88, pp. 5051, 1988.
- [14] LEBEDEV, V.-I., D.-N. LAUIKOV, "A quadrature formula for a sphere of the 131st algebraic order of accuracy," *Dokl. Akad. Nauk*, vol. 366, no. 6, pp. 741-745, 1999.
- [15] LEFEBVRE-LEPOT, A., B. MERLET, T.-N. NGUYEN, "An accurate method to include lubrication forces in numerical simulations of dense Stokesian suspensions," *J. Fluid Mech.*, vol. 769, pp. 369-386, 2015.
- [16] NÉDÉLEC, J.-C., *Acoustic and electromagnetic equations*. Springer-Verlag. 2001, New York. ISBN 0-387-95155-5.
- [17] TEMAM, R., *Navier-Stokes equations. Theory and numerical analysis*. North-Holland Publishing Co. 1977, Amsterdam. ISBN 0-7204-2840-8.
- [18] TRAN, M.-P., NGUYEN, T.-N., "A spectral decomposition in vector spherical harmonics for Stokes equations," *Proceedings of the 1st International*

conference on Applied Mathematics in Engineering and Reliability, pp.337-242, 2016.

About Authors

Minh-Phuong TRAN received her Ph.D. degrees in Applied Mathematics from the University of Orléans, Orléans, France, in 2012. In 2013, she joined the Department of Mathematics and Applications in Ecole Normale Supérieure, Paris, France, as a Postdoctoral Researcher. And in 2014, she became a Lecturer in Faculty of Mathematics-Statistics in Ton-Duc-Thang university, HCMC, Vietnam. Her current research interests include Numerical Analysis, Image Processing, Inverse Problem in Imaging, Computational Fluid Dynamics, Ordinary and Partial Differential Equations.

Thanh-Nhan NGUYEN received his Ph.D. degree in Applied Mathematics from École Polytechnique, Paris, France, in 2013. He is working in Department of Mathematics, Ho Chi Minh City University of Education, HCMC, Vietnam. His current research interests include Ordinary and Partial Differential Equations, Numerical Analysis, and Computational Fluid Dynamics.

"This is an Open Access article distributed under the terms of the Creative Commons Attribution License, which permits unrestricted use, distribution, and reproduction in any medium, provided the original work is properly cited (CC BY 4.0)."