Direct evaluation of lubrication forces in asymptotically corrected completed double layer boundary integral equation formulations

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Abstract

The quality of the solution in completed double layer boundary integral equation formulations for the simulation of densely packed suspensions of rigid particles is poor, due to the inability of the method to capture the lubrication flow between surfaces in near-contact. It is possible to correct this shortcoming by combining the solution of the boundary integral equation with the analytical asymptotic solutions for two-particle problems. The method in principle is applicable to simulations involving many rigid particles. The main difficulty in the implementation of this concept is that the corrective lubrication forces are not known \textit{a priori}. However, the correction forces are related in a linear fashion to the relative velocities of the particles, and thus can be incorporated in the matrix that results from the discretization and numerical solution of the CDL-BIE. The iteration for the correction forces thus becomes part of the iterative solution procedure. The lubrication forces between particles in a pair should be solely a function of the relative motion of the particles, and not of their absolute motion, which depends on the choice of reference frame. The manipulation of the lubrication formulation to ensure frame independence is shown. Finally, a preconditioner based on the structure of the matrix can be applied to reduce the computational effort. The improvement in performance, both in terms of accuracy of the results and computational effort, that can be attributed to the correction algorithm is demonstrated by a set of standard static and dynamic benchmarks. Implications of the results for the treatment of large problems are discussed. Further developments necessary to render the method truly general are also suggested.
1 Introduction

The determination of the macroscopic properties of highly packed suspensions of rigid particles requires the imposition of a deformation on a representative volume element (RVE) of suspension, generally containing hundreds or thousands of particles, depending on the solids volume fraction. Typically, particles are discretized with hundreds of elements, resulting in dense linear systems of dimensions ranging from hundreds of thousands to millions. The solution of such linear systems can be accelerated by using multipole acceleration in combination with iterative non-symmetric solvers such as the generalized minimal residual method (GMRES). A necessary condition for success is a relatively small condition number.

The completed double layer boundary integral equation (CDL-BIE) satisfies these criteria when the velocity on all surfaces is known. In the mobility problem, where the forces and torques applied to the particles are known, but not the velocity, it is possible to manipulate the equations such that well-posedness is restored. Thus, large-scale simulations leading to macroscopic property predictions appear possible. Sadly, at moderate to high solids concentrations, benchmark tests where the macroscopic properties are known empirically show that the simulations fail to provide accurate predictions. The viscosity is underpredicted, while relative velocities between particles are overpredicted. In hindsight, this is not surprising. As shown in a recent simulation by Stokesian Dynamics [7] for a suspension of monomodal spheres, the pair distribution function peaks at particle separations smaller than $1 \times 10^{-3}$ of the particle radius $a$, for volume fractions $\phi > 0.20$. Considering that the size of the RVE is typically on the order of 10$a$, the numerical method is required to resolve a range of length scales of over four decades.

In fact, the treatment of surfaces in close proximity is a known problem in boundary element methods. The flow that results from certain components of the relative motion of two opposing surfaces is singular, and cannot be treated adequately with numerical approximations of reasonable refinement. Fortunately, in the case of spheres the ratio of whose radii is arbitrary, moving through a viscous fluid with known velocities, the force on a particle due to the combined motion of the two particles can be calculated using a set of analytical expressions obtained by various researchers [3].

In this paper, a procedure for incorporating the analytical lubrication forces into the general framework of the CDL-BIE is described briefly. The procedure does not alter the size or block structure of the linear system, which can be solved using the same methodology of the regular CDL-BIE. However, the structure of one of the submatrices is altered significantly, resulting in the need for a revised preconditioner to restore the original diagonal dominance of the system. Secondly, a procedure for extracting the forces on the particles due to lubrication forces only, and thus only a function of the relative motion of the two particles, is described. This also ensures the frame invariance of the lubrication force associated with any particle pair is described. Several static and dynamic benchmarks demonstrate that the lubrication correction is very effective in improving the predictions of particle motion when particles are in close proximity.
2 The corrected boundary integral equation

The CDL–BIE for the case of $n$ rigid particles in an unbounded fluid [6] can be modified, to account for the presence of interparticle forces due to the lubrication flow between nearly-touching surfaces, by incorporating these forces in the range completer, to yield:

$$\frac{1}{2} \varphi(x) + \int_{\Gamma_k} K(x, y) \varphi(y) d\Gamma_k - u^k - \omega^k \times r^k(x) =$$

$$-u_\infty(x) - \sum_{p=1}^{n} \left\{ \left[ F^p - \frac{1}{2} (T^p \times \nabla) \right] + \sum_{q=N_p(1)}^{N_p(N_p)} \left[ \left( F_{\text{orig}}^{pq} - F_{\text{mod}}^{pq} \right) - \frac{1}{2} \left( T_{\text{orig}}^{pq} - T_{\text{mod}}^{pq} \right) \times \nabla \right] \right\} \cdot \frac{G(x - y^k)}{8\pi},$$

where $x$ is on the surface of the $k$th particle, $\Gamma_k$. The equation contains the usual integral operator, the rigid body motion of particle $k$, $u^k + \omega^k \times r^k(x)$, the underlying flow field, $u_\infty(x)$ and the range completer to account for forces $F^p$ and torques $T^p$ applied to each particle $p$. The lubrication correction forces $F_{\text{orig}}^{pq} - F_{\text{mod}}^{pq}$ and torques $T_{\text{orig}}^{pq} - T_{\text{mod}}^{pq}$ are the result of the close-range interaction of each particle $p$ with its neighbor $q$. The subscripts ‘orig’ and ‘mod’ refer to the original and modified geometric representation of particle $q$ which are used to remove the lubrication force predicted by the numerical solution of the BIE for a modified geometry and replace them with the lubrication forces and torques for the original geometry [4]. Both lubrication forces are calculated using analytical expressions. The modified geometry $\bar{\Gamma}_k$ is similar to the original geometry, except that the minimum distance between the surfaces of particle $k$ and its neighbors is such that the numerical solution of the BIE is sufficiently accurate.

The correction forces and torques are not known a priori. However, they are related to the particle velocities linearly. Consider a local coordinate system as illustrated in Fig. 1, where the direction $e_3$ is aligned with the line of centers, while the other two axes are oriented to form a right-handed set. In this coordinate system, it is possible to express the forces and torques on the particles due to their velocity and rate of rotation using relatively simple expressions, corresponding to rotation about an axis normal to the line of centers (mode I), translation along an axis normal to the line of centers (mode II), rotation about an axis along the line of centers (mode III), and translation along the line of centers (mode IV). Any relative motion can be decomposed into a combination of these four basic motions.

For example, rotation of two particles $p$ and $q$ in the $e_3$ direction results in a force on particle $p$ in the $e_2$ direction, which can be expressed as:

$$\bar{F}_{2p}^I = -6\pi \mu r_p \left[ \tilde{\omega}_3 \rho p f_1^I(\kappa, \varepsilon) + \tilde{\omega}_3 q r_p f_2^I(\kappa^{-1}, \varepsilon \kappa^{-1}) \right],$$

where $\mu$ is the viscosity of the fluid, $r_p$ is the radius of particle $p$, $\kappa$ is the ratio $r_q/r_p$ and $\varepsilon$ is the minimum distance between particle surfaces normalized by $r_p$. The
overbar indicates that the quantities are expressed in terms of the local coordinate system. The functions $f_1^I$ and $f_2^I$, where the subscript indicates the object particle (1) or the neighbor particle (2), while the superscript denotes the mode of motion, depend solely on the geometry. For example,

$$f_1^I(\kappa, \varepsilon) = \frac{-2\kappa^{-2}(1 + 4\kappa^{-1})}{15(1 + \kappa^{-1})^2} \log(\varepsilon) + \frac{86 + 166\kappa^{-1} - 66\kappa^{-2} + 64\kappa^{-3}}{375(1 + \kappa^{-1})^3} \varepsilon \log \varepsilon. \quad (3)$$

Note that the coefficient contains a singular term of order $\log(\varepsilon)$, as do the coefficients for mode II motion. Mode III motion is not singular, while mode IV motion contains a leading singularity of order $\varepsilon^{-1}$.

When all modes of relative motion are accounted for, a linear system results, of the form:

$$\begin{align*}
\mathbf{F}_{\text{orig}}^{pq} - \mathbf{F}_{\text{mod}}^{pq} &= \mathbf{F}_{v}^{pq,p} \mathbf{v}_p + \mathbf{F}_{v}^{pq,q} \mathbf{v}_q + \mathbf{F}_{\omega}^{pq,p} \mathbf{\omega}_p + \mathbf{F}_{\omega}^{pq,q} \mathbf{\omega}_q, \\
\mathbf{T}_{\text{orig}}^{pq} - \mathbf{T}_{\text{mod}}^{pq} &= \mathbf{T}_{v}^{pq,p} \mathbf{v}_p + \mathbf{T}_{v}^{pq,q} \mathbf{v}_q + \mathbf{T}_{\omega}^{pq,p} \mathbf{\omega}_p + \mathbf{T}_{\omega}^{pq,q} \mathbf{\omega}_q,
\end{align*} \quad (4) \quad (5)$$

where $\mathbf{T}$ and $\mathbf{F}$ are $3 \times 3$ matrices. Noting that the velocities and forces, expressed in local coordinates, can be expressed in terms of global coordinates by means of a rotation matrix, the following system is obtained:

$$\begin{align*}
\mathbf{F}_{\text{orig}}^{pq} - \mathbf{F}_{\text{mod}}^{pq} &= \mathbf{F}_{v}^{pq,p} \mathbf{v}_p + \mathbf{F}_{v}^{pq,q} \mathbf{v}_q + \mathbf{F}_{\omega}^{pq,p} \mathbf{\omega}_p + \mathbf{F}_{\omega}^{pq,q} \mathbf{\omega}_q, \\
\mathbf{T}_{\text{orig}}^{pq} - \mathbf{T}_{\text{mod}}^{pq} &= \mathbf{T}_{v}^{pq,p} \mathbf{v}_p + \mathbf{T}_{v}^{pq,q} \mathbf{v}_q + \mathbf{T}_{\omega}^{pq,p} \mathbf{\omega}_p + \mathbf{T}_{\omega}^{pq,q} \mathbf{\omega}_q, 
\end{align*} \quad (6) \quad (7)$$

where, for example, $\mathbf{F}_{v}^{pq,p} = (\mathbf{R}^{pq})^{-1} \mathbf{F}_{v}^{pq,p} \mathbf{R}^{pq}$, in which the rotation matrix $\mathbf{R}^{pq}$ transforms a vector in the global coordinate system to the local coordinate system for particle pair $pq$. The evaluation of the lubrication correction matrices can be
implemented with little difficulty, even on a parallel computer. The matrices are then easily assembled into the coefficient matrix for the CDL–BIE, following the structure dictated by Eq. 1. It is also noted that the block structure of the corrected CDL–BIE (CCDL–BIE) matrix is unchanged from the structure of the CDL–BIE matrix, and thus the solution of the matrix can be obtained with the same solver, namely a GMRES algorithm. Before obtaining the solution, two matters must be addressed, frame invariance and preconditioning, as outlined in the following two sections.

3 Matrix manipulation for frame invariance

It is postulated that the lubrication correction must be solely a result of the relative motion between two particles in a pair. Inspection of the expressions for coefficients such as those presented in Eq. 3 reveals that the expressions yield the total forces acting on a spherical particle in the presence of the other particle, and not just the forces due to the lubrication flow between particles. All effects other than those resulting from the lubrication flow must be stripped from the formulation. One possible method for doing so is by altering the expressions for the calculation of the coefficients at the source.

Another possibility is to ensure that the forces yielded by the multiplication of the particle velocities with the lubrication matrices are independent of the translation or rotation of the reference frame. Consider first a translating frame of reference. Its effect can be removed by subtracting the centroid velocity \( \mathbf{v}_c \) from the velocity of the each particle in the pair. For simplicity, the case of two identical particles is considered, however similar considerations can be made for an arbitrary size ratio \( \kappa \). Clearly, only the matrices that multiply the velocity vectors are affected by this manipulation, since angular velocities are unaltered by a translating reference frame. Thus, the term \( F_{v,P}^{pq} \mathbf{v}_p + F_{v,Q}^{pq} \mathbf{v}_q \) in Eq. 6 is replaced with \( F_{v,P}^{pq} (\mathbf{v}_p - \mathbf{v}_c) + F_{v,Q}^{pq} (\mathbf{v}_q - \mathbf{v}_c) \). Given that, for two equal particles, \( \mathbf{v}_c = (\mathbf{v}_p + \mathbf{v}_q)/2 \), it is easy to show that:

\[
F_{v,P}^{pq} (\mathbf{v}_p - \mathbf{v}_c) + F_{v,Q}^{pq} (\mathbf{v}_q - \mathbf{v}_c) = \left[ F_{v,P}^{pq} - \left( \frac{F_{v,P}^{pq} + F_{v,Q}^{pq}}{2} \right) \right] \mathbf{v}_p \\
+ \left[ F_{v,Q}^{pq} - \left( \frac{F_{v,P}^{pq} + F_{v,Q}^{pq}}{2} \right) \right] \mathbf{v}_q.
\]

(8)

The torque matrices are treated identically.

The second type of motion which does not generate any lubrication force, and which corresponds to frame invariance with respect to a rotating frame of reference, is the motion of a rigid dumbbell. Consider two particles, \( p \) and \( q \), with relative velocity \( \mathbf{v}_r = \mathbf{v}_q - \mathbf{v}_p \), and separated by a distance \( \mathbf{r} \). The part of \( \mathbf{v}_r \) which is normal to \( \mathbf{r} \) is given by:
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\[
\mathbf{v}_r^n = \mathbf{v}_r - \left( \mathbf{v}_r \cdot \frac{\mathbf{r}}{r} \right) \frac{\mathbf{r}}{r} = \left[ I - \frac{\mathbf{rr}^T}{r^2} \right] \mathbf{v}_r = \mathbf{S} \cdot \mathbf{v}_r,
\]

(9)

where \( r \) is the magnitude of \( \mathbf{r} \). The angular velocity \( \omega_d \) which, when combined with \( \mathbf{v}_r^n \), constitutes a rigid dumbbell motion, can be related to \( \mathbf{v}_r^n \) by:

\[
\omega_d = \frac{\mathbf{r} \times \mathbf{v}_r^n}{r^2} = \frac{\mathbf{r}}{r^2} \times \mathbf{S} \cdot \mathbf{v}_r = \mathbf{D} \cdot \mathbf{v}_r,
\]

(10)

where the coefficients of the matrix \( \mathbf{D} \) can be obtained with some tensor algebra.

Now, the term \( F_{wp}^{pq} \omega_p + F_{wq}^{pq} \omega_q \) in Eq. 6 is replaced by \( F_{wp}^{pq}(\omega_p - \omega_d) + F_{wq}^{pq}(\omega_q - \omega_d) \). By substituting the results of Eq. 10, the removal of the dumbbell angular velocity can be expressed in terms of quantities which appear explicitly in the matrix equations, namely:

\[
F_{wp}^{pq} \omega_d + F_{wq}^{pq} \omega_d = -(F_{wp}^{pq} + F_{wq}^{pq}) \mathbf{D} \mathbf{v}_p + (F_{wp}^{pq} + F_{wq}^{pq}) \mathbf{D} \mathbf{v}_q.
\]

(11)

Similar treatment is given to the torque equation. Thus modified, the lubrication correction matrices produce lubrication forces that are frame invariant, while remaining in terms of quantities that are part of the original solution vector.

### 4 Preconditioning

The structure of the CCDL–BIE remains similar to the structure of the regular CDL–BIE for the mobility problem, namely:

\[
\begin{bmatrix}
\frac{1}{2}1 + \mathcal{K} & \mathbf{U} \\
\mathbf{F} & 0
\end{bmatrix}
\begin{bmatrix}
\phi \\
\mathbf{v}
\end{bmatrix}
= 
\begin{bmatrix}
\mathbf{s} \\
\mathbf{f}
\end{bmatrix},
\]

(12)

where the block \( 1/2 + \mathcal{K} \) results from the integral operator, the block \( \mathbf{U} \) from the rigid body motion and the lubrication correction, and the block \( \mathbf{F} \) from the equations used to constrain the eigenmodes of the integral operator on the particle surfaces. Previous work [5] has shown that a left preconditioner of the form:

\[
\mathbf{P} = \begin{bmatrix}
\frac{1}{2}1 & \mathbf{U} \\
\mathbf{F} & 0
\end{bmatrix}^{-1}
\]

(13)

is a good approximation to the inverse of the mobility matrix and is very effective at restoring the diagonal dominance of the CDL–BIE. The application of the preconditioner on a vector is equivalent to:

\[
\begin{bmatrix}
\frac{1}{2}1 & \mathbf{U} \\
\mathbf{F} & 0
\end{bmatrix}^{-1}
\begin{bmatrix}
\mathbf{x}_1 \\
\mathbf{x}_2
\end{bmatrix}
= 
\begin{bmatrix}
-U(\mathbf{FU})^{-1}[2\mathbf{F}\mathbf{x}_1 - \mathbf{x}_2] + 2\mathbf{x}_1 \\
\frac{1}{2}(\mathbf{FU})^{-1}[2\mathbf{F}\mathbf{x}_1 - \mathbf{x}_2]
\end{bmatrix}.
\]

(14)
It is readily apparent that the formation and inversion of the matrix $F_U$ is the most computationally expensive operation in the preconditioning process. The off–diagonal blocks for the CCDL–BIE, $F$ and $U$, take the form:

$$
F = \begin{bmatrix}
F^1 & & \\
& F^2 & \\
& & \cdots \\
& & & F^n
\end{bmatrix}, \quad U = \begin{bmatrix}
U^{11} & U^{12} & \ldots & U^{1n} \\
U^{21} & U^{22} & \ldots & U^{2n} \\
& \cdots & \cdots & \cdots \\
U^{n1} & U^{n2} & \ldots & U^{nn}
\end{bmatrix},
$$

(15)

where each submatrix $U^{ij}$ has dimension $M^4 \times 6$.

The preconditioner calculation becomes substantially more complex in the CCDL–BIE than in the regular CDL–BIE. The matrix $U$ is potentially fully populated because all particles (except for isolated ones) are subject to lubrication correction forces from their neighbors, which must be accounted for in the range completer, as can be inferred from Eq. 1. The product $FU$ is also a fully populated matrix, of dimension $6n \times 6n$. Its inversion can be evaluated serially or in parallel, depending on the dimensions of the problem. The preconditioning process is discussed in more detail elsewhere, as is its effectiveness [4].

5 Benchmark and results

The benchmarks chosen to test the above formulation have a twofold purpose. First, they must demonstrate the accuracy of the formulation under a variety of conditions. Second, they must verify that frame invariance is indeed achieved. The first benchmark concerns the interaction of two particles in a linear shear field. The analytical solution for this case was first obtained by Batchelor and Green [1]. An approximation of this solution was obtained more recently by da Cunha and Hinch [2]. The latter solution is used here as a benchmark for the CCDL–BIE code, since it exemplifies the type of simulation that the method is intended for.

In this case, the shear field is described by $v_1 = x_2$. The particles are located at initial positions $(-5.0,0.1,0.0)$ and $(5.0,-0.1,0.0)$ in one case, and $(-5.0,0.5,0.0)$ and $(5.0,0.3,0.0)$ in the other. The relative motion of the two particles should be identical, since the flow field experienced by the particles in the second case is equivalent to the flow field experienced in the first case, as viewed from a reference frame moving with a velocity $v_1 = -0.4$. The relative trajectories are shown in the leftmost panel of Fig. 2, where the semi–analytical results obtained using da Cunha and Hinch’s procedure are also plotted. Within numerical error, the two CCDL–BIE results are identical to each other. In addition, they are very close to the semi–analytical trajectory, in contrast to the case for the uncorrected CDL–BIE, where the dynamic simulation results in the interference of the particle surfaces.

The second benchmark simulates two particles located in a fluid in rigid body rotation, which is equivalent to a stationary flow as viewed from a rotating frame of reference. The angular position of the particles, and the gap between them, are plotted against the angular position of the dumbbell formed by the two particles. The plot shows that all angular positions are equal, as expected. As expected,
Figure 2: Minimum surface distance $\varepsilon$ as a function of relative angular position $\theta$ for two particles interacting in a shear flow $v_1 = x_2$, where the starting particle positions in case 2 are shifted by 0.4 in the $x$ direction, compared to the semi-analytical solution (left); angular position of the particles and minimum separation as a function of the doublet angular position in a fluid undergoing rigid-body motion.

also the inter–particle gap remains constant, confirming the independence of the correction method of a rotating reference frame.

The overall effect of the lubrication correction should be measured in terms of the performance, which can be defined as the ratio of the error versus the computational cost. The preconditioner has the effect of reducing the number of GMRES iterations required to obtain a solution within a given tolerance. In the regular CDL–BIE, when two surfaces approach each other the discretization is refined to improve the accuracy of the calculation, resulting in the generation of very small elements belonging to different surfaces and in close proximity to each other. A side effect of this is a decrease in the convergence rate of the iterative solution. With the lubrication correction, the distance between neighboring surface always exceeds or equals a specified minimum value, and the convergence rate remains much faster, even for the same number of elements, as shown in Fig. 3. In addition, the lubrication correction results in much higher accuracy without the requirement for excessively fine discretizations. High accuracy, combined with faster and fewer GMRES iterations, result in a factor of 1000 to 10000 improvement in performance.

6 Discussion and conclusions

A procedure that corrects the error in a boundary element calculation due to poor resolution of various singular flows located between surfaces in near–contact is demonstrated. The implementation of the correction is such that the structure of the resulting linear system is the same as that of the original CDL–BIE formulation, except for the entries of the matrix that corresponds to the particle velocities.
Figure 3: Number of GMRES iterations required to obtain a ratio of current to initial residual of $10^{-7}$ with CDL–BIE and CCDL–BIE, as a function of the number of elements (left), and relative error as a function of computational time for a mode IV motion with a gap of $10^{-3}a$ on a Compaq XP1000 workstation (right).

This difference requires the modification of the preconditioner that was originally used for the CDL–BIE.

By construction, the method is frame invariant, and the correction forces are due only to the relative motion between the particles, as is shown in various benchmark problems. The benchmarks also show that the accuracy of the numerical results is excellent, and that is is now possible to study microscale effects, such as surface roughness or solvation forces, within a mesoscale simulation. The ability to cover several length scales was not present in the uncorrected CDL–BIE or similar methods.

The lubrication correction was made possible by the existence of analytical or semi-analytical expressions relating the motion of two spherical particles to the forces experienced by these. In theory, this would limit the applicability of the correction procedure to spherical particles. In practice, if it is possible to approximate the surfaces in near-contact with spherical surfaces characterized by an effective radius, then any particle or container geometry could be treated, since the numerical method would treat the non-spherical surfaces away from the lubrication flow region.

In the case that the surfaces in near-contact cannot be represented by spherical surfaces, but they are still smooth, it becomes necessary to obtain analytical expressions for shapes of more general application, such as randomly oriented ellipsoids. This challenging problem will require the collaboration of mathematicians, but will lead to a an efficient and robust procedure for treating multiple length scales simultaneously for completely arbitrary geometries.
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