A corrected BEM for the inclusion of near-field effects associated with suspension flows at low Reynolds numbers

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Abstract

In suspensions of rigid spheres at high solids fractions, a large portion of the particles are in near-contact with their neighbors. In such cases, near-field interactions play an important role in the particle trajectories. The prediction of these trajectories therefore hinges on a correct representation of the near-field interactions. It is shown in this study that traditional BEM techniques do not capture near-field interactions adequately, with unpredictable effects on the resulting trajectories.

A methodology for combining analytical near-field interactions with numerical BEM solutions is described. The methodology is benchmarked against known semi-analytical solutions. It is found that lubrication interactions are accounted for with good accuracy, resulting in accurate trajectory predictions even for very small inter-particle distances. Using this method, it becomes possible to study the effect of sources of irreversibility (such as surface roughness) in a fully quantitative sense.

1 Introduction

Suspensions of rigid particles are found in many natural and synthetic processes. The simplest model of such systems is a suspension of rigid spheres of equal size suspended in a Newtonian fluid. When the solids fraction is large, the particle structure becomes anisotropic and the macroscale rheology of the suspension non-Newtonian. It is well-known that the particle structure is intimately linked to the rheology [1, 14]. One of the principal reasons for performing numerical simulations is that the particle locations are known with great accuracy, along with the
volume averaged stress corresponding to any given configuration. Hence, the link between particle structure and rheology can be made.

A recent illustration of this concept is provided by Sierou and Brady [13], who use Stokesian Dynamics (SD) to investigate the pair distribution function that results from shearing a representative volume element of a suspension of monomodal particles, for volume fractions ranging from 0.10 to 0.60. It is found that, in the case of a velocity in the x direction and a velocity gradient in the y direction, the pair distribution function in the xy plane cannot be described solely by r, as in the dilute limit. This is found to coincide with increasingly strong normal stress differences $N_1$ and $N_2$.

The Stokesian dynamics approach has been used successfully to make qualitative and quantitative predictions concerning the rheology of concentrated suspensions. However, it suffers from some drawbacks. First, only spherical particles can be treated. Second, while near-field and far-field interactions are accounted for, the intermediate field is not. Third, it is difficult to treat walls - these have to be approximated by an array of spheres.

The flow of suspensions of rigid particles has been simulated using various boundary element methods (BEM) by many researchers [6, 11]. The BEM offers several attractions, in particular the ability to treat any desired geometry with little difficulty, the absence of approximations (save for the unavoidable one due to surface discretization), and the convergence rate of the solutions. Unfortunately, for highly concentrated suspensions the BEM cannot be relied upon to provide accurate results due to the difficulty in resolving the lubrication flow in regions of near-contact between surfaces [9].

In this work, a newly developed method for correcting the inaccuracy in the near-field solution associated with the BEM is presented. In essence, the method is a combination of SD for the near-field and BEM for the intermediate and far-field. The goal of this study is to perform a dynamic simulation of the interaction of two particles, and to compare the resulting trajectories with analytical solutions. A successful outcome will result in a methodology for obtaining particle structures that is both flexible and accurate.

2 Numerical formulation

Given velocity boundary conditions, the completed double layer boundary integral equation (CDL–BIE) formulation is a Fredholm equation of the second kind. The numerical solution of such equations by boundary discretization gives rise to diagonally dominant systems [8], which can be solved effectively using iterative techniques, such as GMRES [12]. This is essential for the solution of large problems. Using multipole acceleration, the operation count to obtain the solution for a given configuration is of $O(N \log N)$.

In the CDL–BIE, the velocity $\mathbf{u}$ at a point $x \in \Gamma$, where $\Gamma = \Gamma_1 \cup \Gamma_2 \cup \ldots \Gamma_n$
is the union of all individual particle surfaces, can be written as:

$$u(x) = u_\infty(x) - \frac{1}{2} \phi(x) + \int_{\Gamma} K(x, y) \cdot \phi(y) d\Gamma_y$$

$$+ \sum_{p=1}^{n} \left[ \frac{F^p - \frac{1}{2} (T^p \times \nabla)}{8\pi} \right] G(x, y^p)$$

(1)

where $F^p$ and $T^p$ are the known force and torque applied to particle $p$; $u_\infty(x)$ is the velocity that would exist at location $x$ in the absence of particles due to an underlying flow field; $K$ is the kernel function:

$$K_{ij}(x, y) = \frac{3}{4\pi} \frac{(x_i - y_i)(x_j - y_j)(x_k - y_k) n_k(y)}{r^5},$$

(2)

where $r = |x - y|$. The double layer representation can only describe the flow field due to force- and torque-free particles. A Stokes doublet originating at points $y^p$ in the interior of each particle is used to complete the flow field. The Stokeslet $G$ is given by:

$$G_{ij}(x) = \left( \frac{\delta_{ij}}{R} + \frac{x_i x_j}{R^3} \right),$$

(3)

where $R = |x - y^p|$. On the surface of particle $p$, the velocity is given by:

$$u(x) = u^p + \omega^p \times r^p.$$  

(4)

Finally, the rank deficiency of the system is removed by setting:

$$F^p = \int_{\Gamma_p} \phi(x) d\Gamma,$$

$$T^p = \int_{\Gamma_p} \phi(x) \times r^p(x) d\Gamma.$$  

(5)

(6)

When the minimum gap between particle surfaces is on the order of 5% of the radius, the error in the relative velocity between the two particles becomes very large. One of the consequences of this is that the relative position of the particles cannot be calculated accurately, resulting in an erroneous outcome of interactions between particles. The effect that this has on the accuracy of the calculated particle structure is not known.

Analytical solutions for the interactions between two particles have been obtained for the set of relative particle motions shown in Fig. 1 [2, 10]. Any relative motion between two particles can be decomposed into a linear combination of these basic motions.

Consider first motion of type I, for two particles aligned in the $x_1$ direction. Particle A, of radius $r_A$, rotates about an axis through its center parallel to the $x_3$ direction with angular velocity $\omega_A^l$ and particle B, of radius $r_B$, rotates about an axis through its center parallel to the $x_3$ direction with angular velocity $\omega_B^l$. The
flow field set up by the particles’ motion results in forces on each particle along the \( x_2 \), and couples in the \( x_3 \) direction, given by:

\[
\begin{align*}
F_A^I &= -6\pi \mu r_A \left\{ \omega_A r_A f_A^I(k, \epsilon) - \omega_B r_B f_B^I(k^{-1}, \epsilon k^{-1}) \right\}, \\
F_B^I &= -6\pi \mu r_B \left\{ \omega_A r_B f_B^I(k, \epsilon) - \omega_B r_B f_B^I(k^{-1}, \epsilon k^{-1}) \right\}, \\
T_A^I &= -8\pi \mu r_A^2 \left\{ \omega_A r_A t_A^I(k, \epsilon) - \omega_B r_B t_B^I(k^{-1}, \epsilon k^{-1}) \right\}, \\
T_B^I &= -8\pi \mu r_B^2 \left\{ \omega_A r_B t_B^I(k, \epsilon) - \omega_B r_B t_B^I(k^{-1}, \epsilon k^{-1}) \right\},
\end{align*}
\]  

where \( k = r_B/r_A, \epsilon = d/r_A \), with \( d \) taken as the inter-particle gap (the minimum distance between the spherical surfaces). The coefficients \( f_i^I(\kappa, \epsilon) \) and \( t_i^I(\kappa, \epsilon) \) should be interpreted as follows: the subscript \( i \) is 1 if the affecting particle, for which the force or couple is being calculated, is the same as the affecting particle, the motion of which generates the force or couple, 2 otherwise. The superscript refers to the relative motion mode (I in this case); \( \kappa \) is the reciprocal of the ratio of the radius of the affecting particle to the radius of the other particle, and \( \epsilon \) is the ratio of the inter-particle gap to the radius of the affecting particle. For example, in the first equation in the above set, \( f_A^I(k, \epsilon) \) represents the force on particle A due to its own rotation combined with the presence of particle B, normalized by the Stokes force of the same isolated particle moving in an infinite fluid with speed \( \omega_A r_A \). The values of the coefficients \( f_i^I(\kappa, \epsilon) \) and \( t_i^I(\kappa, \epsilon) \) can be calculated using the asymptotic solutions for small inter-particle gaps developed by Jeffrey and Onishi [7].

In the case of mode II relative motion, with particle A moving in the \( x_2 \) direction with velocity \( v_A^{II} \) and particle B moving in the \( x_2 \) direction with velocity \( v_B^{II} \),
the flow field applies forces to each particle in the \( x_2 \) direction, and couples in the \( x_3 \) direction. These are given by:

\[
F_{A}^{II} = -6\pi \mu r_{A} \left\{ v_{A}^{II} f_{1}^{II}(k, \epsilon) + v_{B}^{II} f_{2}^{II}(k^{-1}, \epsilon k^{-1}) \right\}, \\
F_{B}^{II} = -6\pi \mu r_{B} \left\{ v_{A}^{II} f_{2}^{II}(k, \epsilon) + v_{B}^{II} f_{1}^{II}(k^{-1}, \epsilon k^{-1}) \right\}, \\
T_{A}^{II} = -8\pi \mu r_{A}^2 \left\{ v_{A}^{II} t_{1}^{II}(k, \epsilon) + v_{B}^{II} t_{2}^{II}(k^{-1}, \epsilon k^{-1}) \right\}, \\
T_{B}^{II} = 8\pi \mu r_{B}^2 \left\{ v_{A}^{II} t_{2}^{II}(k, \epsilon) + v_{B}^{II} t_{1}^{II}(k^{-1}, \epsilon k^{-1}) \right\}.
\] (8)

Again, the results of Jeffrey and Onishi can be used to calculate the coefficients \( f_{II} \) and \( t_{II} \).

In mode III motion, the particles rotate about their line of centers, in the \( x_1 \) direction. The angular velocities of particles A and B are \( \omega_{A}^{III} \) and \( \omega_{B}^{III} \) respectively. As before, only the couple due to the relative motion of the particles, \( \omega_{AB}^{III} \), is of interest. The resultant couples in the \( x_1 \) direction are given by:

\[
T_{A}^{III} = -8\pi \mu r_{A}^2 \left\{ \omega_{A}^{III} r_{A} t_{1}^{III}(k, \epsilon) \right\}, \\
T_{B}^{III} = -8\pi \mu r_{B}^2 \left\{ \omega_{A}^{III} r_{B} t_{2}^{III}(k, \epsilon) \right\}.
\] (9)

The coefficients \( f_{III} \) and \( t_{III} \) are given by Jeffrey and Onishi [7].

Finally, in mode IV the spheres approach each other along their line of centers. In the case illustrated above, the spheres A and B are aligned in the \( x_1 \) direction, with velocities \( v_{A}^{IV} \) and \( v_{B}^{IV} \). As before, only forces generated by relative motion are of interest. These are in the \( x_1 \) direction, and their magnitudes are given by:

\[
F_{AB}^{IV} = -6\pi \mu r_{A} \left\{ v_{AB}^{IV} f_{1}^{IV}(k, \epsilon) \right\}, \\
F_{BA}^{IV} = -6\pi \mu r_{B} \left\{ v_{AB}^{IV} f_{2}^{IV}(k, \epsilon) \right\}.
\] (10)

Asymptotic solutions for mode IV motion were derived by Cooley and O’Neill [3] for the case where one of the particles is stationary, which corresponds to the relative motion of interest here.

The method for combining the asymptotic solutions with the BEM solution is similar to the procedure adopted by Zinchenko [15] for calculating the effective conductivity of highly loaded composite materials. Consider the evaluation of the boundary integral with respect to a collocation point located on particle A, as shown in Fig. 2. The velocity field caused by the interaction of particles A and B can be approximated by the field caused by the interaction of particle A and a slightly smaller version of particle B. The size of B is reduced to such an extent that the gap between the neighboring surfaces is large enough to allow an accurate BEM solution, as shown in Fig. 2. The lubrication flow that is essentially removed due to the reduction in size of particle B is substituted by correction forces and
Figure 2: Schematic showing the equivalence, with respect to a collocation point on A, of a system of two nearly touching particles A and B with a modified system consisting of particle A and a smaller version of particle B, augmented with correction forces and torques which account for the modified dimensions of B.

torques calculated using Eqns. 7-10. The corrected boundary integral equation can be written as:

\[
\frac{1}{2} \phi(x) + \sum_{p=1}^{n} \int_{\Gamma_p} K(x, y) \phi(y) d\Gamma y - u^k - \omega^k \times r^k = \\
\underline{u}_\infty(x) - \sum_{p=1}^{n} \left[ F_p^p - \frac{1}{2} (T_p^p \times \nabla) \right] \cdot \frac{G(x, y^p)}{8\pi} \\
- \sum_{j=1}^{N(k)} \left\{ (F_{\text{org}}^{kj} - F_{\text{mod}}^{kj}) - \frac{1}{2} \left[ (T_{\text{org}}^{kj} - T_{\text{mod}}^{kj}) \times \nabla \right] \right\} \cdot \frac{G(x, y^k)}{8\pi},
\]

where \( \Gamma \) is a modified boundary, similar to the original boundary except that the neighbors of the particle which owns the collocation node are shrunk; \( N(k) \) is the number of neighboring particles to \( k \). The force \( F_{\text{org}}^{pj} \) and \( F_{\text{mod}}^{pj} \) represent the analytical lubrication forces for the original and modified geometry applied to particle \( p \) by its neighbor \( j \). The torques are treated similarly.

Since the correct velocities are not known \textit{a priori}, the correction forces are also unknown. Therefore, iteration is necessary to satisfy the system, with the first step in the iteration consisting of the uncorrected solution. A Newton–Raphson algorithm is used to determine the corrective forces and torques.

3 Test problem and results

The aim of the corrected BEM formulation is to obtain accurate particle trajectories. Thus, a benchmark is required to assess the validity of the method. The analytical solution for the interaction of two particles in an otherwise empty shear
field, as illustrated in Fig. 3, was first obtained by Batchelor and Green [1]. Subsequently, da Cunha and Hinch [4] developed an approximate solution by using curve fits for the infinite series solutions of Batchelor and Green. The trajectories are calculated using an Adams predictor-corrector ODE solver (LSODE).

The analytical trajectories for particle B, whose center is initially located at \((-10, \Delta y)\), are shown in Fig. 4. Note that for certain values of \(\Delta y\) the trajectories appear to collapse onto one. This is not so. A plot of the trajectories in the region of near-contact, also shown in Fig. 4, indicates that although the trajectories become extremely close to one another, they remain distinct.

The extremely close spacing of the trajectories when the particles are passing one another makes the accuracy of the solution critical for the purposes of obtaining accurate dynamic simulations. If the velocity solution is in error in this region of closely-spaced trajectories, the outcome of the interaction could be significantly compromised due to error-induced trajectory jumping. In fact, this ef-
fect is thought by many [1, 4, 5] to be responsible for the irreversible behavior observed in many experiments.

The trajectory of particle B obtained using an unaided BEM simulation, with and without adaptive mesh refinement, for $\Delta y = 0.1$, is shown in Fig. 5. Significant deviation is observed in both cases. The trajectory predicted with the fixed mesh (96 elements per particle) begins to diverge from the analytical solution at a separation of $\approx 20\%$ of the particle radius, and the two particles intersect at $\theta \approx -2.7$. The trajectory predicted with the adaptive mesh (up to 1300 elements per particle) begins to diverge at a separation of $\approx 5\%$ of the particle radius, and particle interference occurs when $\theta \approx -2.5$.

On the other hand, the trajectory predicted with the corrected BEM simulation follows the analytical trajectory rather closely at all relative positions. A slight amount of noise can be observed for very small separations, $\varepsilon < 1 \times 10^{-4}$. This can be corrected by reducing the tolerance for the iterative calculation of the correction forces and torques, at the expense of increased computational cost.

Finally, a few remarks concerning numerical aspect of the calculation should be made. The iterative calculation of the corrective forces and torques requires multiple solutions of the BEM problem at a given configuration, versus only one solution in the case of the traditional BEM. However, when surfaces are very close to one another, with correspondingly refined mesh, the number of GMRES iterations to achieve a given tolerance increases. On the other hand, the condition number of the 'corrected' problem is low, and the number of GMRES iterations remains small. For the present calculations, particles were shrunk so that the minimum distance between surfaces was 4% of the particle radius. For these conditions, the number of GMRES iterations for the corrected BEM was approximately 20, versus 150 for the uncorrected BEM. Thus, overall the correction does not produce additional computational cost while the accuracy is improved tremendously.

4 Conclusions

Dynamic simulations with the unaided BEM cannot be relied upon to provide accurate predictions of the particle structure because of the inability of the method to capture the lubrication flow between nearly touching surfaces. The particles inevitably intersect, with unpredictable effects. Lubrication solutions can be incorporated into the simulation in a seamless manner by adopting a technique used previously for the calculation of the steady-state effective conductivity of highly loaded composites. The techniques has been modified so that the surface modification is a function of the location of the collocation node. Thus, the (inaccurate) near-field interactions are corrected, while the (accurate) far-field interactions are left unaltered.

The method results in very accurate trajectories in an absolute sense. While obtaining such accuracy is still computationally expensive, the method described here makes it achievable using finite resources. In practice, the simulation described here would be extremely difficult to replicate experimentally. Typically,
Figure 5: Inter-particle gap as a function of relative angular position of particle B for an initial relative position of (-10,0.1), calculated using uncorrected (left) and corrected (right) BEM.

spheres of \( \approx 5 \times 10^{-3} \) m radius are used in experimental work. Assuming that a surface can be considered smooth if the size of its asperities is less than one tenth of the size of the gap, then for the smallest gaps considered here, the asperity size would be \( \approx 20 \times 10^{-9} \) m, a high polish indeed.

The main outcome of this work is that the error inherent in the simulation has been reduced to such a point that it is much smaller than one would expect from physical parameters such as surface roughness. As a result, it is now possible to introduce sources of irreversibility in a controlled manner. Any irreversibility that is observed can now be attributed to the introduced source, rather than to error inherent in the simulation method. As a consequence, this methodology represents a significant step forward in the study of macrostatistical irreversibilities.

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References


