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A singularity method for calculating hydrodynamic forces and particle velocities in low-Reynolds-number flows

By T. DABROS†
Department of Chemistry, McGill University, Montreal, Quebec, Canada, H3A 2A7

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A numerical technique is presented which allows one to estimate hydrodynamic forces and torques or translational and angular velocities of particles in a general flow field. Particle–solid wall interactions can be readily included. The base functions used in the technique presented are singular fundamental solutions of the Stokes equation for a point force and a point source. The least-square approach is used preferentially in order to find the intensities of these singularities. Test calculations show that the results are self-consistent and in fairly good agreement with the exact solutions in a wide range of conditions. For example, for a spherical particle moving with no slip towards the solid wall, it has been shown that the method can provide good estimates of the resistance coefficient up to separations of the order of 5 % of the particle radius. We believe that better agreement, for smaller separations, is within reach at the expense of increased computer costs. For spheroidal particles good results were obtained for aspect ratio in the range 0.5–2.0.

1. Introduction

Knowledge of hydrodynamic forces acting on particles is essential in any attempt to analyse the mass transfer or rheological properties of colloidal systems. Until now only some dilute systems of particles of simple shape could be considered as well described in the sense that an exact analytical solution of the Stokes equation is available. However, even for spherical particles, problems important for the kinetics of particle deposition, such as interactions between particles deposited onto a solid wall and particles freely suspended in a flow, have not been solved owing to a lack of symmetry required to solve these problems in an analytical manner. Generally speaking, the solution of the Stokes equation can be found in an analytical form for any of the orthogonal reference systems if the geometry of the considered particles is such that coordinate surfaces fit the physical boundaries of the problem. Good examples of this approach include the classic problem of a spherical particle in a uniform flow, solved by Stokes (1851), and ellipsoidal or two spherical particles in a linear flow discussed by Stimson & Jeffery (1926). In more complicated cases a number of approximate treatments are possible; e.g. an extensive theory exists to describe behaviour of slender bodies (e.g. Burgers 1938; Cox 1970; Batchelor 1970; Russell *et al.* 1977; Liron 1978, Liron & Mochon 1976*b*). The approach is based on the distribution of singularities and their higher moments along the slender body in such a way that appropriate boundary conditions at the surface of the body are fulfilled, at least approximately.

† On leave from Jagiellonian University, Cracow, Poland.

Chwang & Wu (1974, 1975) and Chwang (1975) have explored the fundamental singular solution of the Stokes equation to obtain solutions for several specific body shapes translating and rotating in a viscous fluid. Some rules regarding the type and method of distributing the singularities have been given as conclusions of these papers. From a generalization of observations for various axisymmetrical bodies placed in a variety of linear and quadratic flows it was found that (i) the flow alone determines the necessary types of singularities, (ii) the distribution range of all singularities seems to depend solely on body geometry, and (iii), if the solution for a flow of reduced degree $\partial V/\partial x_i$ ($i = 1, 2, 3$) requires certain singularities, then the x_i derivatives of these singularities are needed to construct the solution associated with the flow V. Regarding the distribution range of the singularities, it was pointed out that some results for plane-symmetric bodies in a potential flow may also be valid in all types of Stokes flow. By providing the exact solution of the Stokes equation in an elegant, closed form, the singularity method proved to be a useful alternative to the more standard methods of solution. Unfortunately one cannot, in a straightforward manner, generalize this approach to systems of many particles or to particles in the vicinity of a wall.

In a series of papers, Gluckman, Pfeffer & Weinbaum (1971) and Gluckman, Weinbaum & Pfeffer (1972) developed a new method for treating the slow viscous motion past finite assembles of particles of arbitrary shape, termed the multipole representation technique. The approach is based on the theory that the solution for any object conforming to a natural coordinate system in a particle assemblage can be approximated by a truncated series of multi-lobular disturbances in which the accuracy of the representation is systematically improved by the addition of higher-order multipoles. For example, for a system of spherical particles the solution is found in terms of Legendre functions. Taking advantage of the symmetry of the system, it is possible to eliminate a number of the terms of the general solution. The remaining coefficients can then be determined using the boundary collocation principle, namely one can require that the no-slip boundary condition for a given number of surface points on each sphere be satisfied. If the infinite series is truncated to yield a proper number of coefficients, a determined system of linear equations can be found which allows one to calculate the unknown coefficients. Usually, a fast convergence to the exact solution is observed as the number of boundary points is increased, provided that some principles are met regarding the distribution of the collocation points. In the case of two spherical particles settling in an arbitrary orientation under gravity, Gantos, Pfeffer & Weinbaum (1978) noted that, while a given configuration of points produces good results over a certain range of relative positions, the same set of points could produce substantial errors outside this region. Therefore, the distribution of the points over the particle surface must be carefully tested in every case in order to avoid so-called ill-conditioning problems. In general the method is useful and, from a numerical point of view, it provides a fast way of estimating the hydrodynamic forces and velocities of particles for a variety of systems (Leichtberg, Weinbaum & Pfeffer 1976; Gantos *et al.* 1978; Gantos, Weinbaum & Pfeffer 1980; Dagan, Weinbaum & Pfeffer 1982*a*). However, every system requires derivation and careful analysis of the base functions.

Although, in principle, both methods discussed can be generalized to purely three-dimensional problems, little has been done in this field owing to the complexity of the problem.

Youngren & Acrivos (1975) used the boundary-element method to calculate hydrodynamic forces and torques acting on spheroidal and cylindrical particles in a uniform and simple shear flow. The solution of the Stokes equations was expressed in the form of linear integral equations for the Stokeslets distribution over the particle surface. The required density of the Stokeslets, identical with the surface stress forces, can be obtained numerically by reducing the integral equations to a system of linear algebraic equations. The technique has been successfully tested against the analytical solutions for spheroidal particles in a shear flow. Rallison & Acrivos (1978) applied a similar method in order to determine the deformation and condition of break-up in shear of a liquid drop suspended in another liquid of different viscosity. This very general method, which can be used in the case of bodies of arbitrary shape, so far has not been used to analyse flow fields around systems of particles.

The objective of this paper is to show some results of an attempt to find hydrodynamic forces and velocities of arbitrarily shaped particles, placed in an arbitrary flow field, particularly in the vicinity of the wall, using a singular point solution as the base function. The strength of the singular forces and sources situated inside each particle will be found in such a way that the appropriate boundary conditions at the particle surface will be fulfilled, at least approximately. As one can see, the method presented belongs to the same family as the three methods discussed above. Singular fundamental solutions of the Stokes equation are used to find the flow field for a given system. The method has points in common with the multipole representation technique due to the fact that both methods can be considered as boundary-collocation or boundary-least-square approaches. The technique presented is general in the sense that we deny ourselves any advantages of simplifications related to the symmetry of the particular system. However, if the system contains elements of symmetry, the amount of computations can be reduced in a straightforward manner.

The organization of the paper is as follows. In §2 we shall discuss the general background of the method with a short presentation of the formulae used later on. In §3, results will be given of calculations of hydrodynamic forces and torques acting on particles. The method of calculating particle velocities will be discussed in §4. Finally, in §5, we shall present a discussion and summarize the conclusions of the paper. Most of the calculations shown in this paper have been carried out in order to estimate the range of applicability of the method, especially for strong particle–particle or particle–wall interactions.

2. Formulation of the problem

We shall consider the flow field satisfying the Stokes equation

$$\mu \nabla^2 u_i = \frac{\partial p}{\partial x_i}, \tag{1}$$

and the continuity equation
$$\nabla \cdot \boldsymbol{u} = 0, \tag{2}$$

where $\boldsymbol{u} = (u_1, u_2, u_3)$ is the velocity vector defined in a Cartesian coordinate system x_1, x_2, x_3, ; p is the pressure and μ the dynamic viscosity of the fluid. In an unbounded fluid a flow disturbance produced by a point force $\boldsymbol{f}(\boldsymbol{y})$ acting at $\boldsymbol{y} = (y_1, y_2, y_3)$ can be expressed in terms of velocity components and pressure as (Lamb 1953):

$$v_i(\boldsymbol{x}) = t_{ij}(\boldsymbol{x}, \boldsymbol{y})\, f_j(\boldsymbol{y}), \quad p(\boldsymbol{x}) = g_j(\boldsymbol{x}, \boldsymbol{y})\, f_j(\boldsymbol{y}), \tag{3a, b}$$

where
$$t_{ij} = \frac{1}{8\pi\mu}\left(\frac{\delta_{ij}}{r} + \frac{r_i r_j}{r^3}\right), \tag{4}$$
$$g_j = \frac{1}{4\pi}\frac{r_j}{r^3}, \tag{5}$$

with $r_i = x_i - y_i$, $r = (r_i r_i)^{\frac{1}{2}}$ and δ_{ij} the Kronecker delta. The exact solution for a force singularity, as noted by Blake (1971) and Blake & Chwang (1974), in the presence of a stationary plane boundary $x_3 = 0$ with the no-slip boundary condition, can be expressed by (3) with t_{ij} and g_i given by:

$$t_{ij} = \frac{1}{8\pi\mu}\left[\left(\frac{\delta_{ij}}{r} + \frac{r_i r_j}{r^3}\right) - \left(\frac{\delta_{ij}}{R} + \frac{R_i R_j}{R^3}\right) + 2h(\delta_{j\alpha}\delta_{\alpha k} - \delta_{j3}\delta_{3k})\frac{\partial}{\partial R_k}\left\{\frac{hR_j}{R^3} - \left(\frac{\delta_{i3}}{R} + \frac{R_i R_3}{R^3}\right)\right\}\right], \tag{6a}$$

$$g_i = \frac{1}{4\pi}\left[\frac{r_j}{r^3} - \frac{R_j}{R^3} - 2h(\delta_{j\alpha}\delta_{\alpha k} - \delta_{j3}\delta_{3k})\frac{\partial}{\partial R_k}\left(\frac{R_3}{R^3}\right)\right], \tag{6b}$$

where $\alpha = 1, 2$; $h = y_3$ and $R = [(x_1 - y_1)^2 + (x_2 - y_2)^2 + (x_3 + y_3)^2]^{\frac{1}{2}}$. The solution for a point source, with mass outflow q in unit time in an unbounded fluid, can be expressed as

$$u_i = \frac{q}{4\pi} s_i, \tag{7}$$

where
$$s_i = \frac{r_i}{r^3}. \tag{8}$$

In the presence of a stationary plane boundary $x_3 = 0$, s_i is given by (Blake & Chwang 1974)

$$s_i = \left(\frac{r_i}{r^3} + \frac{R_i}{R^3}\right) - 2\left(\frac{R_i}{R^3} - \frac{3R_i R_3 R_3}{R^5}\right) + 2h\left(\frac{\delta_{i3}}{R^3} - \frac{3R_i R_3}{R^5}\right). \tag{9}$$

For unbounded systems, higher moments of the singularities can easily be found by differentiation. As was pointed out by Blake & Chwang (1974), this method cannot be applied when a boundary is present. However, in principle the same effect as produced by higher moments of the singularities can be obtained by a proper distribution of the fundamental ones.

Consider a system of N groups, each consisting of M force and source singularities. Due to the linearity of the Stokes equation, the disturbance of velocity at point $\boldsymbol{x}$ can be expressed quite generally as

$$v_i(\boldsymbol{x}) = \sum_{mn} t_{ij}(\boldsymbol{x}, \boldsymbol{y}_{mn}) f_j(\boldsymbol{y}_{mn}) + \sum_{mn} s_i(\boldsymbol{x}, \boldsymbol{y}_{mn}) q(\boldsymbol{y}_{mn}), \tag{10}$$

where $\boldsymbol{y}_{mn}$ denotes the position vector of the mth singularity ($m = 1, 2, \ldots, M$) in the nth group ($n = 1, 2, \ldots, N$).

Let S_n denote the surface confining the nth group of the singularities and let $\boldsymbol{x}^{sn'}$ be one of the S points situated at $S_{n'}$. If $S_{n'}$ is identified with the surface of the solid body, the velocity of the $\boldsymbol{x}^{sn'}$ point can be expressed as

$$\boldsymbol{u}(\boldsymbol{x}^{sn'}) = \boldsymbol{u}^{0n} + \boldsymbol{\omega}^{n'} \times \boldsymbol{r}^{sn'}, \tag{11}$$

where $\boldsymbol{u}^{0n'}$ and $\boldsymbol{\omega}^{n'}$ are translational and angular velocities respectively and $\boldsymbol{r}^{sn'}$ is the surface position vector measured with respect to the origin of the particle. The difference between $\boldsymbol{u}(\boldsymbol{x}^{sn'})$ and the fluid velocity, where the fluid velocity consists of the disturbance velocity given by (10) and external flow field $V(x)$, which itself satisfies the Stokes equation, can in general be expressed as:

$$D_i(x^{sn'}) = u_i^{0n'} + \epsilon_{ijk}\,\omega_j^{n'}\,r_k^{sn'} - \sum_{mn} t_{ij}(x^{sn'}, y_{mn})\,f_j(y_{mn}) - \sum_{mn} s_i(x^{sn'}, y_{mn})\,q(y_{mn}) - V_i(x^{sn'}), \quad (12)$$

where ϵ_{ijk} is the unit isotropic triadic. When the no-slip boundary conditions are appropriate, $D_i(x^{sn'})$ should be identically zero for every point on each particle surface. In principle this can be achieved by a proper distribution of the singularities in the vicinity of the centre (or the centreline in the case of slender bodies) of each particle. For a spherical particle placed in an unbounded uniform flow, it suffices to place the singular force and source doublet in the centre of the particle to obtain zero velocity at the sphere surface. In this case the intensity of the singular force is exactly $6\pi\mu a V_x$ (a being the particle radius and V_x the velocity of the uniform flow). The source doublet intensity is equal to $F_x a^2/6\mu$.

As was shown by Cox & Brenner (1967), the velocity disturbance produced by an arbitrary body can be presented in the form of a multipole expansion. This is equivalent to having singular forces, force doublets, quadrupoles, etc. placed in the particle centre. Intensity of the poles is uniquely determined by the hydrodynamic forces acting at the particle surface. The question arises as to whether or not these intensities can be determined uniquely from the boundary conditions imposed on the system. From integral solutions of the Stokes equation, it follows that this is true in principle. However it is not obvious that the same is true for any arbitrary distribution of a limited number of singularities inside the particle. Therefore one may expect that the method will give reasonable estimates of the hydrodynamic forces for a given distribution of singularities as long as the flow field is not too complicated. In order to find the range of applicability of the technique presented, we will discuss a number of test calculations for which exact solutions of the Stokes equation exist.

Once an optimum distribution of forces has been found, one can calculate the force and torque exerted on the particle. The total force is equal to

$$F^n = \sum_m f(y_{mn}), \quad (13)$$

and the torque of the nth particle can be calculated as

$$T^n = \sum_m r^f(y_{mn}) \times f(y_{mn}), \quad (14)$$

where $r^f(y_{mn})$ is a local component of the force position vector.

In order to obtain a better insight into the method, we would like to return to the question of how the singular point solution can be used to find an approximate solution in some simple cases. Burgers (1938) has shown that a singular solution (3) can be used to find the Stokes formula for the resistance of a sphere. If the spherical particle is held at a uniform velocity with components $(V_x, 0, 0)$, in order to keep it stationary one has to exert a force upon the sphere in the negative x-direction. Disturbances produced by such a sphere will not differ much from that produced by a single point force acting at the origin provided that we are a certain distance away from the origin and that the direction and magnitude of the forces are the same. In order to find the force acting on the sphere we may look for intensities of the singular force such that the mean value of the resultant flow velocity $V_x + u_x, u_2, u_3$ will vanish.

Here u_i is given by

$$u_i = t_{ij} f_j.$$

Writing this explicitly

$$(V_x + u_x)_{\text{mean}} = \frac{1}{4\pi a^2}\int_S (V_x + u_x)\,\mathrm{d}S = V_x + \frac{f_x}{8\pi\mu}\frac{4}{3a} = V_x + \frac{f_x}{6\pi\mu a},$$

where a is a sphere radius. The term $(V_x + u_x)_{\text{mean}}$ vanishes if $f_x = -6\pi\mu a V_x$. Thus the Stokes formula is obtained by considering the mean values of the velocity components over the sphere surface.

Burgers also showed (1938) that the proper expression for the spherical particle in parabolic flow can be deduced in a similar way. Tam (1969) has used the point-force approximation to obtain the correction factor to the Stokes equation for two spherical particles in a uniform flow. Analytical formulae which were obtained agree with the exact solution of Jeffery for separations larger than a few particle radii, but even for two spheres in contact the error was below 9 %. We shall generalize this approach to deal with arbitrarily distributed particles in the vicinity of a wall. A number of singularities will be used in order to obtain more accurate solutions of the problem in the cases of non-spherical particles or strong particle–wall interactions.

3. Hydrodynamic drag on particles

3.1. *One singular force approximation*

Let us consider N spherical particles with centres at $\boldsymbol{x}_1, \boldsymbol{x}_2, \ldots, \boldsymbol{x}_N$ placed in an external flow $V(\boldsymbol{x})$, which itself satisfies both the Stokes and continuity equations. By generalizing Burgers' approach, if a singular point force acts at the centre of each particle, we may look for intensities of the forces such that the integral

$$\int_{S_{n'}} \Big(V_i(\boldsymbol{x}_{n'}) - \sum_n t_{ij}(\boldsymbol{x}_{n'}, \boldsymbol{y}_n) f_j(\boldsymbol{y}_n)\Big)\,\mathrm{d}S = 0 \tag{15}$$

will vanish. This equation leads directly to a system of linear equations

$$\sum_n G_{ij}(\boldsymbol{x}_{n'}, \boldsymbol{y}_n) f_j(\boldsymbol{y}_n) = b_i(\boldsymbol{x}_{n'}), \tag{16}$$

where

$$b_i(\boldsymbol{x}_{n'}) = \int_{S_{n'}} V_i(\boldsymbol{x}_{n'})\,\mathrm{d}S, \tag{17}$$

$$G_{ij}(\boldsymbol{x}_{n'}, \boldsymbol{y}_n) = \int_{S_{n'}} t_{ij}(\boldsymbol{x}_{n'}, \boldsymbol{y}_n)\,\mathrm{d}S. \tag{18}$$

The surface integrals (17) and (18) were calculated numerically using an 8th-order numerical formula of the Gaussian type (Abramowitz & Stegun 1964). In order to check the method, a number of test calculations were conducted. First, as expected, the calculations yield proper results for single spherical particles in an unbounded fluid. Figure 1 shows the drag correction factor $\lambda = F_x/6\pi\mu a V_x$ for the Stokes formula for a system of two spheres in a uniform flow. The solid line represents the exact solution of Jeffrey, while the dashed line shows the result obtained using the present method. The points were calculated by introducing more singularities in each particle, as discussed in §3.2. It can be seen that a good agreement between exact and approximate values of the correction factor is observed even if only one singular point

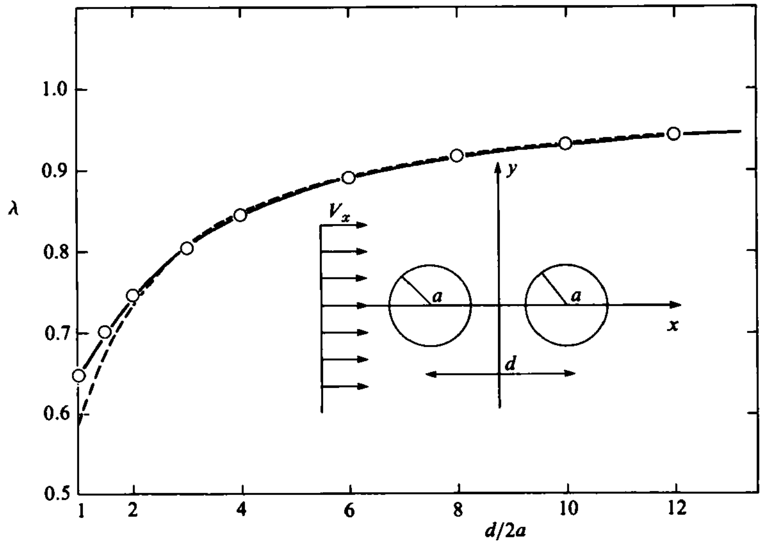

FIGURE 1. Drag correction factor for two spheres in a uniform flow as a function of their separation $d/2a$.

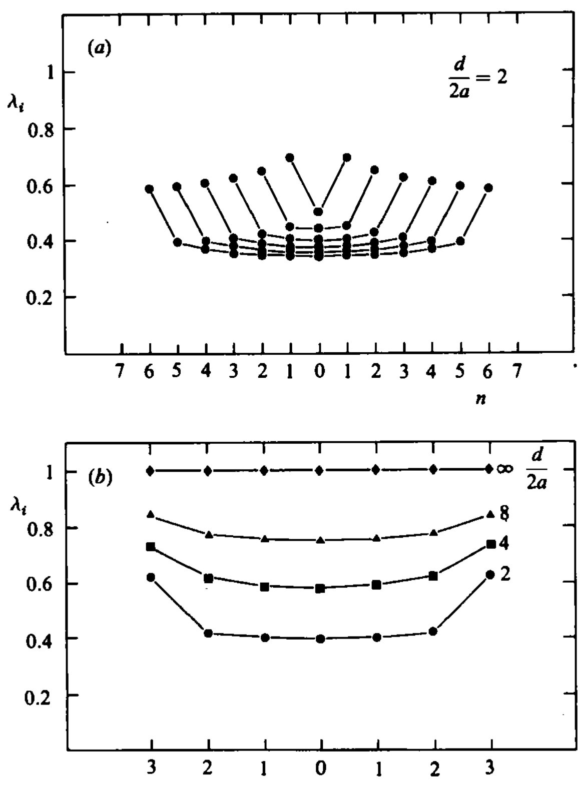

FIGURE 2. (*a*) Drag correction factor λ_i for chains containing different numbers of spheres with $d/2a = 2$. (*b*) Drag correction factor λ_i for a seven-sphere chain at different sphere spacings.

is used for $d/2a > 2$. For two spheres in contact the error is 9%. Similar calculations were performed for linear systems of spherical particles. Results are shown in figure 2. It should be noted that the solid lines which connect the points have no physical meaning, as the drag correction factor λ_i has a discrete value for each sphere. Corrections determined for chains containing various numbers of spheres at spacing $d/2a = 2$ can be compared with results of Gluckman *et al.* (1971) which were obtained by use of the multipole collocation technique. The maximum error of these calculations was estimated at 2.5%. The maximum difference between Gluckman *et al.* and results presented here occurs for the three-particle system and is 8%. For larger separations the difference becomes negligible. Taking into account the simplicity of the prescribed technique and the fact that it can be used for any spatial distribution of particles, one can see the advantage over other methods, especially when only approximate information on drag forces is required.

Figure 3 shows results of calculations for linear aggregates of spherical particles in contact. The calculations were performed for uniform flow, either perpendicular (curve 1) or parallel (curve 2) to the aggregate axis. One may expect that the drag on such systems should not differ very much from that on an elongated spheroid or cylinder. In particular, for a spheroid with semi-axes a and b (with b measured along the symmetry axis), Oberbeck's formula (Lamb 1953) for uniform flow in the direction of the symmetry axis leads to a force of magnitude

$$F_s = 16\pi\mu a V_x \left[-\frac{2\left(\frac{b}{a}\right)}{\left(\frac{b}{a}\right)^2 - 1} + \frac{2\left(\frac{b}{a}\right)^2 - 1}{\left[\left(\frac{b}{a}\right)^2 - 1\right]^{\frac{3}{2}}} \ln\left(\frac{\frac{b}{a} + \left[\left(\frac{b}{a}\right)^2 - 1\right]^{\frac{1}{2}}}{\frac{b}{a} - \left[\left(\frac{b}{a}\right)^2 - 1\right]^{\frac{1}{2}}} \right) \right]^{-1}. \tag{19}$$

For large b/a this formula reduces to

$$F_s = 4\pi\mu b V_x \frac{1}{\ln\left(\frac{2b}{a}\right) - 0.5}. \tag{20}$$

For a finite circular cylinder, Burgers (1938) obtained the formula

$$F_s = 4\pi\mu b V_x \frac{1}{\ln\left(\frac{2b}{a}\right) - \alpha_1}, \tag{21}$$

where $\alpha_1 = 0.72$, b is the semi-length, and a the radius of the cylinder. Curves 3 and 4 in figure 3 show the correction factors

$$\lambda_s = \frac{F_s}{6\pi\mu a V_x} \tag{22}$$

calculated from formula (20) and (21) respectively. As one can see, the correction factors calculated for a system of spheres lie between the curves obtained for cylindrical and spheroidal particles with similar geometry. When particles are oriented perpendicular to the uniform flow the theoretical expressions for a long cylinder and spheroid are the same (Burgers 1938) and can be expressed as

$$F_\mathrm{J} = 8\pi\mu b V_x \frac{1}{\ln\left(\frac{2b}{a}\right) + 0.5}. \tag{23}$$

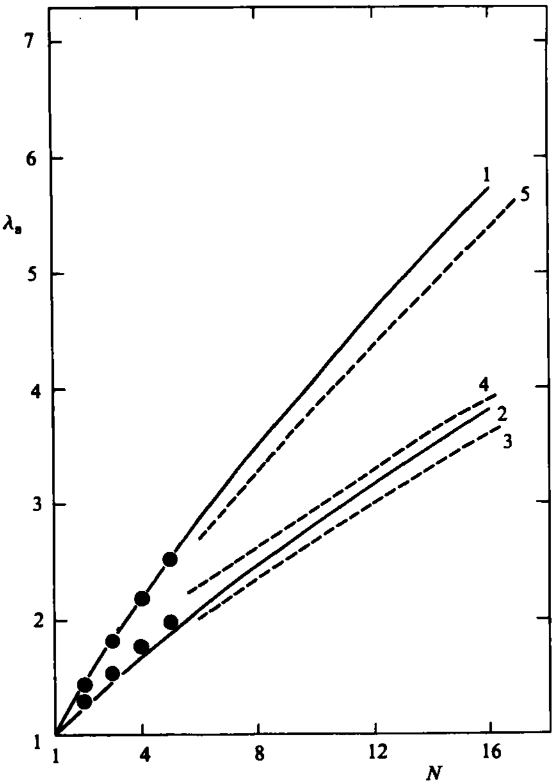

FIGURE 3. Dimensionless resistance force $\lambda_s = F_x/6\pi\mu a\, V_x$ of a straight chains of N spheres in a uniform flow: curve 1, chain perpendicular to the flow; curve 2, chain parallel to the flow; curves 3 and 5 show calculated resistance of spheroidal and cylindrical particles in proper orientations; points, experimental data of Horvath (1974).

The forces calculated for linear systems of spheres appear to be about 6 % higher than those predicted for finite cylinders and spheroids (curve 5). Dots on figure 3 show experimental values of the correction factors obtained by Horvath (1974). Excellent agreement between experimental and theoretical values is obtained when the aggregate is oriented perpendicular to the flow. For parallel orientation an error of 5–8 % is observed. Both experimental and theoretical calculations show that the presence of a solid wall may have a significant influence on the settling rate of long aggregates. In fact, for $h/a = 60$, the correction factor accounting for wall interaction for a single sphere, is equal to 1.9 %. Our calculations show that, for 15 spheres in contact moving perpendicularly to the wall, the equivalent correction is about 10 %. When the aggregate is oriented parallel to the wall and moves along its axis, the presence of the wall can change its mobility by 2.3 % compared with 1.2 % for a single particle. When a linear system of 15 spheres moves perpendicularly to the wall along the symmetry axis, the correction factor for $h/a = 60$, where h now describes the position of the central particle, is equal to 5.9 %. All these results can be obtained in a straightforward manner by the presented technique if (6a) is used to describe t_{ij} in (16)–(18).

3.2. *Multiple singularities in every particle*

In order to increase the accuracy of the calculations and to make it possible to find the torque on the particle, let us return to (12), where it was assumed that in every particle M singular forces and M singular sources were present. Let us assume that $D_i(x^{sn'})$ is equal to zero. In order to calculate the drag on the particle, we will assume that the velocity of the particles and the external flow field is known. One obtains therefore a set of $3SN$ linear equations with $3MN$ unknown values of the singular force intensities and MN unknown source intensities. Thus the equation

$$\sum_{mn} t_{ij}(x^{sn'}, y_{mn}) f_j(y_{mn}) + \sum_{mn} s_i(x^{sn'}, y_{mn}) q(y_{mn}) = u_i^{0n'} + \epsilon_{ijk} \omega_j^{n'} r_k^{sn'} - V_i(x^{sn'}), \quad (24)$$

may be written in shorthand notation as $\boldsymbol{Cx} = \boldsymbol{d}$, where $\boldsymbol{x}$ stands for unknown values of the forces and sources intensities, $\boldsymbol{C}$ is a proper matrix which depends on the geometry of the system and $\boldsymbol{d}$ is a vector determined by the external flow and movement of the particle. If $4MN > 3NS$ one obtains an overdetermined system of linear equations which can be solved in a number of different ways, e.g. in such a way that the sum of the squares of the residuals will be minimized. The adopted calculation algorithm was as follows. First, we used one singular point force placed in the particle centre. Using the approach described in §3.1, its optimum value was found. In a second step, at a given number of surface points of every particle, the value of the discrepancy between the required and approximate value of the velocity was calculated and by solving the overdetermined system of equations the intensities of the singular forces and sources were calculated using the least-squares method. To do this, in most of the calculations we used subroutine LLSQF of the IMSL library. It is possible that the matrix $\boldsymbol{C}$ may not be of full rank because some columns of $\boldsymbol{C}$ may be linear combinations of other columns due to an inherent symmetry of the system. The linearity-dependent columns were eliminated from the matrix $\boldsymbol{C}$ and a lower-rank problem was subsequently solved. In order to determine the rank of the matrix a tolerance parameter τ must be defined. During calculation, column pivoting was performed to introduce columns of $\boldsymbol{C}$ one at a time into the basis. At each step the column that produced the larger reduction of the residual sum of squares was selected. The process was terminated if inclusion of the next column would result in a matrix with condition number greater than or equal to $1/\tau$ (Lawson & Hanson 1974). For calculations performed with double precision for spherical particles τ was usually equal to 10^{-6}–10^{-8}.

Two other methods of solution of the overdetermined system of linear equations were tested. The first was based on finding the solution which minimizes the maximum absolute value of the residuals (the Chebyshev norm) (Barrodale & Phillips 1975). However, this method failed to find a proper solution in the sense that it did not reflect the expected symmetry of the distributed forces. The second method tested minimized the sum of the absolute values of the residuals (L1 solution, Barrodale & Roberts 1980). Results obtained by means of this method were very close to the least-square solutions. However in some cases, e.g. for small particle–wall separations, rounding errors became significant making the subroutine break down. The efficiency of both Chebyshev's and the L1 method was much less than that of the least-squares method.

In the actual calculations, usually 7–14 singularities distributed symmetrically around the particle centre were used. As a first test let us consider a spherical particle in a uniform and simple shear flow. In this calculation 7 singular forces and sources were used with coordinates $(0,0,0)$, $(\pm b, 0, 0)$, $(0, \pm b, 0)$ and $(0, 0, \pm b)$ relative to the particle centre where b is made dimensionless with respect to the particle radius. Results for various values of b are shown in table 1. As one can see, in the whole range of b the calculated hydrodynamic force remains practically unchanged. Furthermore,

b	F†	Σ_{sq}‡
0.004	1.0000	8.4×10^{-10}
0.01	1.0000	1.1×10^{-8}
0.02	1.0000	1.7×10^{-7}
0.04	1.0000	2.8×10^{-6}
0.08	0.9999	4.5×10^{-5}
0.16	0.9998	7.2×10^{-4}
0.32	0.9988	1.1×10^{-2}
0.64	1.0035	9.4×10^{-2}

† $F = F_{x(\text{calculated})}/6\pi\mu a V_x$.
‡ Σ_{sq} – sum of squares of residuals at 66 surface points of the spherical particle.

TABLE 1. Test calculations for various distributions of singularities

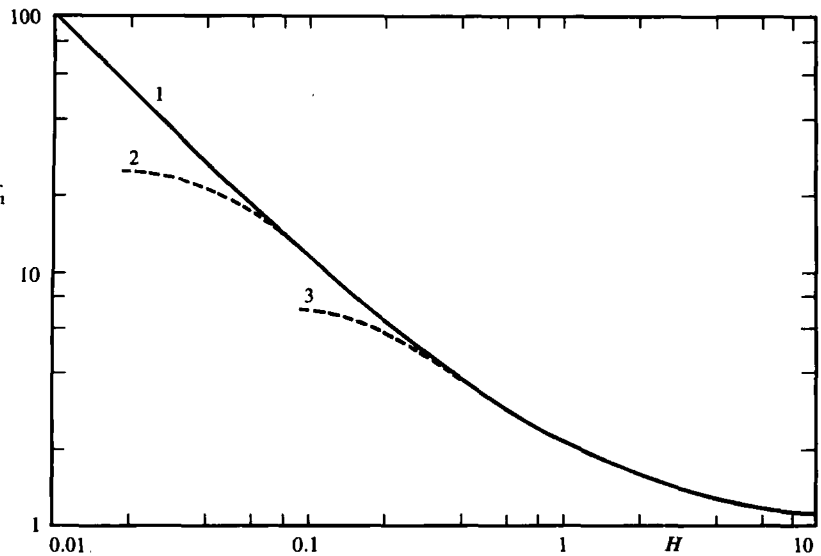

FIGURE 4. *Correction factor to Stokes law for a sphere moving toward the solid wall as a function of particle–wall distance* H: curve 1, exact solution; curves 2 and 3, approximate solution obtained by present technique for various numbers of singular points.

the sum of source intensities is equal to zero within rounding errors in all cases. This reflects the fact that the net production of fluid inside the particle should equal zero. It is worthwhile to note that this condition was not forced on the system artificially during the calculations; rather it reflects the ability of the method to satisfy the proper boundary conditions imposed on the system in a consistent way.

As a second example, let us consider a spherical particle moving towards a solid wall on which we apply the no-slip boundary condition. An exact expression for the correction factor to the Stokes equation $F_z = 6\pi a\mu V_z$ obtained by Maude (1961) and Brenner (1961) is

$$f_1 = \tfrac{4}{3}\sinh\alpha \sum_{n=1}^{\infty} \frac{n(n+1)}{(2n-1)(2n+3)}\left[\frac{2\sinh[(2n+1)\alpha]+(2n+1)\sinh 2(\alpha)}{4\sinh^2[(n+\frac{1}{2})\alpha]-(2n+1)^2\sinh^2(\alpha)}-1\right], \quad (25)$$

in which $\alpha = \cosh^{-1}(H+1)$, where $H = h/a-1$. The dependence of f_1 versus H is shown in figure 4, curve 1. For large H, $f_1 \approx 1+\frac{9}{8}H$ and for small separations when resistance forces are mainly due to squeezing the fluid out of the gap between particle and wall $f \cong 1/H$. Figure 4, curve 3, shows f_1 as a function of H calculated using 13 singular forces distributed symmetrically at $(0,0,0)$, $(\pm b, 0, 0)$, $(0, \pm b, 0)$ and $(0, 0, \pm b)$ with $b = 0.01$ and 0.1. The number of surface points was changed between 26 and 68 without significant influence on the results. As one can see, for particle–wall separations larger than one particle radius, the calculated results are in excellent agreement with the exact ones calculated from (25). For smaller separations the agreement is fairly good for $H > 0.2$; however, the method fails to predict proper values of the coefficient for $H \rightarrow 0$. In fact the calculated values of f_1 are practically constant for $H < 0.05$. The reason for the discrepancy is obviously related to the fact that for small separations almost all resistance is due to squeezing the fluid out of the small gap between the particle and the wall. As noted earlier, one cannot expect that such a small number of singularities will be able to represent properly such a complicated flow field as exists in the vicinity of the particle surface. In fact, when 20 singular points were used with 66 surface points, it was possible to obtain much better agreement even for separations smaller than 10% of the particle radii (curve 2, figure 4). This clearly indicates that the accuracy of the method can be controlled by the number of singular points. However, for what follows we shall usually use 13 or 14 singular points in the calculations in order to show how the method works in such conditions.

As another example, let us consider a stationary spherical particle situated in an axisymmetrical stagnation-point flow given by the equation

$$V_{sr} = A_0(xz\boldsymbol{i}_x + yz\boldsymbol{i}_y - z^2\boldsymbol{i}_z). \tag{26}$$

If the centre of the particle lies on the z-axis, only the F_z component of the force is non-zero owing to symmetry. Following Goren & O'Neill (1971), F_z can be expressed as

$$F_z = 6\pi\mu A_0 a z^2 f_0,$$

where f_0 is the correction factor accounting for hydrodynamic particle–wall interaction. As $h/a \rightarrow \infty$, f_0 approaches unity. Figure 5 shows the dependence of f_0 as a function of H calculated from the exact solution of the Stokes equation (solid line) according to Goren & O'Neill's method. Points represent values obtained using the present technique. In these calculations the number of surface and singular points were 26 and 13, respectively. The limiting value of f_0 as $H \rightarrow 0$, according to the exact solution, is equal to 3.230. The value obtained by the singularity method is 7.5% higher and is equal to 3.470. For separations larger than 10% of the particle radius the difference between exact and calculated values is smaller than 5%, and the error drops below 1% for $H > 0.4$. Similar calculations for a spherical particle in a simple shear flow in the vicinity of the wall show that for $H = 0.1$ the error in the calculations is 3.51% and as $H \rightarrow 0$ grows to 9.0%.

Using the method discussed and taking advantage of the linearity of the Stokes equation, it is possible to calculate particle trajectories in any kind of flow. To do so one has first to calculate the hydrodynamic drag acting on the stationary particle in a specific flow field. Next one calculates all elements of the resistance, torque and coupling tensors for every particle. With this information it is possible to calculate the components of the translational and angular velocities. However such an approach is tedious and inefficient, especially for multiparticle systems. In the next section we wish to discuss a direct method of calculating particle velocities.

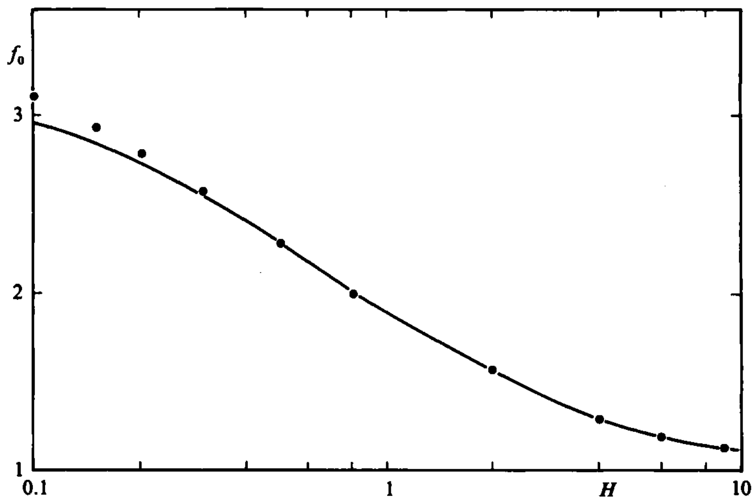

FIGURE 5. Drag correction factor f_0 for a stationary sphere placed symmetrically in a stagnation-point flow as a function of particle–wall separation H: solid line represents exact solution; dots calculated values.

4. Velocities of particles

Consider a system of N particles in an external flow field V. Let F^n_{ext} and T^n_{ext} denote the respective external force and torque acting on the nth particle. Neglecting inertial effects, these forces must be matched by hydrodynamic forces acting on the particles. Taking into account (13) and (14) one can write this condition explicitly as

$$\sum_m f(y_{mn}) = F^n_{\text{ext}}, \tag{27}$$

$$\sum_m r^f(y_{mn}) \times f(y_{mn}) = T^n_{\text{ext}}. \tag{28}$$

Equations (27) and (28) provide $6N$ equations which can be regarded as equality constraints imposed on singular forces and sources. Therefore one can try to minimize a norm $\|D_i(x^{sn'})\|$, where $D_i(x^{sn'})$ is given by (12), in such a way that (27) and (28) are satisfied exactly. Two approaches were used; (i) the method of Lagrangian multipliers; and (ii) a direct least-squares solution of the system of linear equations with linear constraints by orthogonal transformations.

4.1. *Method of Lagrangian multipliers*

In order to simplify the notation, let us denote $D_i(x^{sn'}) = G_k$, where $k = 1, 2, \ldots, 3SN$ is determined by a proper combination of subscripts $i = 1, 2, 3$, $n' = 1, 2, \ldots, N$ and $s = 1, 2, \ldots, S$. Equation (12) can then be written as

$$G_k = C_{kl}\, x_l + d_k, \tag{29}$$

where x_l describes the unknown values of the singular forces (for $1 \leqslant l \leqslant 3MN$) and sources (for $3M+1 \leqslant l \leqslant 4MN$). For $4MN+1 \leqslant l \leqslant 4MN+6N$, x_l denotes the (unknown) values of the translational and angular velocities. The coefficients d_k correspond to the external flow velocities at given surface points of the particles.

The constraints can be expressed as

$$H_\alpha = \sum_\beta E_{\alpha\beta} x_\beta - g_\alpha = 0, \tag{30}$$

where the matrix $E_{\alpha\beta}$ and the vector g_α are determined using (27) and (28). G_k is a function to be minimized with linear constraints $H_\alpha = 0$. Thus one can form a functional

$$\mathscr{F} = \sum_k G_k^2 + \lambda_\alpha H_\alpha, \tag{31}$$

where λ_α are the multipliers. In order to minimize $\mathscr{F}$, its first derivatives with respect to the unknown values of x must equal 0,

$$\frac{\partial \mathscr{F}}{\partial x_\gamma} = 0. \tag{32}$$

This procedure leads to a system of linear equations of the form

$$\sum_l \left(2 \sum_k C_{kl} C_{k\gamma}\right) x_l + \sum_\alpha E_{\alpha\gamma} \lambda_\alpha = -2 \sum_k d_k C_{k\gamma}, \quad \sum_l E_{\alpha l} x_l = g_\alpha, \tag{33}$$

with $4MN$ unknown values of the forces and sources intensities, $6N$ values of translational and angular velocities and $6N$ unknown values of λ.

It is worthwhile to note that information about the external flow field and external forces acting on the particles is necessary to determine the right-hand side of the equation, but this does not influence the matrix on the left-hand side. Since during calculations most of the computer time is spent calculating the coefficients of the matrix, it is possible to solve the problem for various external flow fields and forces after having calculated the values of the left-hand-side matrix once and for all. In this way one can make the calculations more efficient.

4.2. *Results of the Lagrangian multipliers method*

As an example of the applicability of the method let us consider a spherical particle in the vicinity of a wall. We will look for the translational and angular velocities of (i) the sphere in a simple shear flow, and (ii) of the particle undergoing motion due to a constant force acting parallel to the wall. In both cases it will be assumed that the sphere is free to rotate and that no external torques are exerted on it. The calculations were performed with 26 surface points and 7 or 13 singular points distributed exactly as described above.

In simple shear flow, far away from the wall, the sphere follows the fluid streamlines with velocity hG, where h is the distance between the wall and the centre of the particle and G is the shear rate. It will also rotate with angular velocity $\omega_y = \frac{1}{2}G$. As the sphere approaches the solid surface both translational and rotational velocities are damped. Analytically the solution process can be split into two steps as discussed by Goldman, Cox & Brenner (1967). Taking advantage of the linearity of the Stokes equation one can find first the hydrodynamic forces and torques acting on a stationary sphere in a simple shear flow. In the next step, resistance forces acting on the sphere translating and rotating in a quiescent fluid can be found. By combining these results the translational and rotational velocity of the particle can be found. In particular, when external forces and torques are absent, the velocity of the particle is matched in such a way that the sum of the hydrodynamic forces and torques is equal to zero.

Table 2 presents values of u_x^0/Gh and $2\omega_y/G$ for various particle–wall separations

$\frac{h}{a}$	$\left(\frac{u}{hG}\right)_{exact}$ †	$\left(\frac{u}{hG}\right)_{app}$ ‡	error %	$\left(\frac{\omega_y}{\frac{1}{2}G}\right)$ †	$\left(\frac{\omega_y}{\frac{1}{2}G}\right)_{app}$ ‡	error %
∞	1	1	0	1	1	0
10.067	0.9996	0.9997	0.0	0.9995	0.9995	0
2.3524	0.9777	0.9778	0.0	0.9778	0.9776	0.0
1.5431	0.9218	0.9271	0.6	0.9237	0.9286	0.5
1.1276	0.7669	0.8451	10.2	0.7792	0.8744	12.5

† exact solution of Stokes equation.
‡ results obtained by present technique.

TABLE 2. Translational and angular velocities at a sphere moving near a wall in a simple shear flow

using the present technique. Exact values are also given for comparison. As one can see, the error for $h/a > 1.5$ is negligible. As the sphere approaches the wall, the errors grow. Since, as mentioned earlier, the discussed method gives finite values of the resistance coefficient for both perpendicular and parallel movement of the sphere in contact with the wall, the evaluated velocities are overestimated.

During the calculations it was noted that the method reveals some numerical problems for specific positions of the sphere relative to the wall. In these cases the system of linear equations seems to be numerically singular. This problem is especially pronounced for non-spherical particles.

4.3. *Orthogonal transformation method*

The system of linear equations (29) with linear constraints (30) can be solved directly using orthogonal transformations. In principle, one may derive a lower-dimensional unconstrained least-squares problem which can be solved by the method outlined previously. In the next step, the solution of the derived problem can be transferred to obtain the solution of the original problem. Generally speaking, the system of linear equations $\boldsymbol{Ex} = \boldsymbol{g}$ and the overdetermined system of linear equations $\boldsymbol{Cx} = \boldsymbol{d}$, can be found (assuming that matrix $\boldsymbol{E}$ is of order m_1) by finding an orthogonal matrix $\boldsymbol{K}$ which when postmultiplied by $\boldsymbol{E}$ transforms $\boldsymbol{E}$ into a lower triangular matrix. Postmultiplying $\boldsymbol{E}$ and $\boldsymbol{C}$ by $\boldsymbol{K}$ gives

$$\begin{bmatrix} \boldsymbol{E} \\ \boldsymbol{C} \end{bmatrix} \boldsymbol{K} = \begin{bmatrix} \tilde{\boldsymbol{E}}_1 & 0 \\ \tilde{\boldsymbol{C}}_1 & \tilde{\boldsymbol{C}}_2 \end{bmatrix},$$

where $\tilde{\boldsymbol{E}}_1$ is a $m_1 \times m_1$ non-singular lower triangular matrix. This step allows one to find in an easy way the solution $\boldsymbol{y}_1$ of the system of equations $\tilde{\boldsymbol{E}}_1 \boldsymbol{y}_1 = \boldsymbol{d}$. As shown in Lawson & Hanson's book (1975) the solution of the constrained problem is equal to

$$\boldsymbol{x} = \boldsymbol{K} \begin{bmatrix} \boldsymbol{y}_1 \\ \boldsymbol{y}_2 \end{bmatrix},$$

where $\boldsymbol{y}_2$ is a least-square solution of $\tilde{\boldsymbol{C}}_2 \boldsymbol{y}_2 = \boldsymbol{f} - \tilde{\boldsymbol{C}}_1 \boldsymbol{y}_1$. Calculations using this method were based on algorithm LSE presented by Lawson & Hanson (1975).

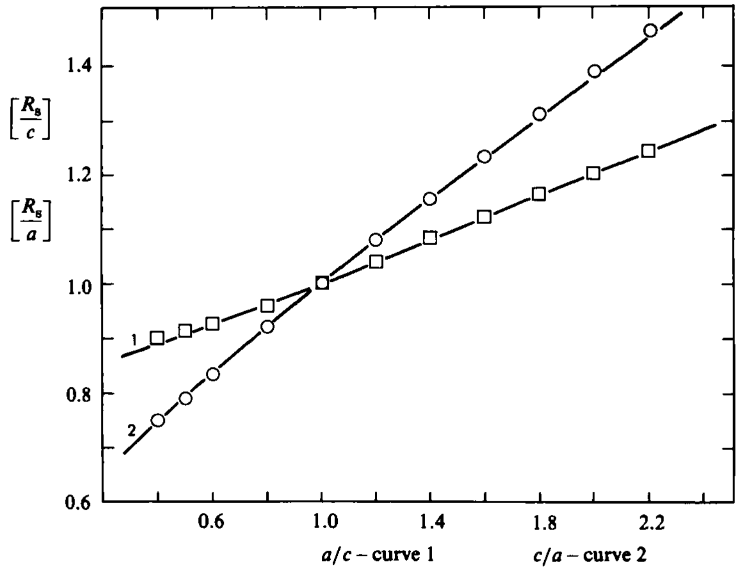

FIGURE 6. Drag on a stationary spheroidal particle in a uniform flow as a function of particle geometry: curve 1, oblate spheroid broadside-on and prolate spheroid end-on; curve 2, oblate spheroid edge-on and prolate spheroid broadside-on.

4.4. *Results of the least-square calculations*

The least-square approach proved to be both universal and trouble free. The algorithm used automatically selected a non-singular basis to the solution, allowing use of a very general numerical scheme without analysis of specific relations between variables such as singular forces, which could eventually exist due to the symmetry of the system. The only parameters which need be defined are: (i) shape of the particles; (ii) their positions; (iii) external forces and torques acting on the particles; and (iv) external fluid-flow field which would exist if the particles were absent. As a result of the calculations the translational and angular velocity of the particles are obtained directly. This allows use of the subroutine to calculate the trajectories of the particles by solving a system of ordinary differential equations:

$$\frac{\mathrm{d}x_i^{0n}}{\mathrm{d}t} = u_i^{0n}, \tag{34}$$

$$\frac{\mathrm{d}\Omega_i^n}{\mathrm{d}t} = \omega_i^n, \tag{35}$$

where x_i^{0n} and Ω_i^n describe spatial and angular positions of the particle respectively.

As an example of the applicability of this method to non-spherical particles, let us consider a spheroidal particle moving in an otherwise quiescent fluid under the influence of a force directed perpendicularly to one of the semi-axes of the particle. The results of the calculations are shown in figure 6. In the case of an ellipsoid of semi-axis a, b, c with a being parallel to the direction of motion, the resistance is the same as that of a sphere of radius R_s given by (Lamb 1953)

$$R_s = \frac{8}{3}\frac{abc}{\chi + \alpha_0 a^2}, \tag{36}$$

where
$$\chi = abc\int_0^\infty \frac{\mathrm{d}\lambda}{[(a^2+\lambda)(b^2+\lambda)(c^2+\lambda)]^{\frac{1}{2}}}, \tag{37}$$
and
$$\alpha_0 = abc\int_0^\infty \frac{\mathrm{d}\lambda}{(a^2+\lambda)^{\frac{3}{2}}[(b^2+\lambda)(c^2+\lambda)]^{\frac{1}{2}}}. \tag{38}$$
In case of a prolate spheroid end-on and an oblate spheroid broadside-on, the semi-axes b and c are equal and the problem reduces to calculation of R_s/c in terms of a/c. Solving (32)–(38) and substitution in (36) yields
$$\frac{R_s}{c} = \frac{\frac{4}{3}\left(1-\frac{a^2}{c^3}\right)^{\frac{3}{2}}}{\left(1-2\frac{a^2}{c^2}\right)\cos^{-1}\left(\frac{a}{c}\right)+\frac{a}{c}\left(1-\frac{a^2}{c^2}\right)^{\frac{1}{2}}} \quad \text{for } \frac{a}{c}<1, \tag{39}$$
and
$$\frac{R_s}{c} = \frac{\frac{4}{3}\left(\frac{a^2}{c^2}-1\right)^{\frac{3}{2}}}{\left(2\frac{a^2}{c^2}-1\right)\cosh^{-1}\left(\frac{a}{c}\right)-\frac{a}{c}\left(\frac{a^2}{c^2}-1\right)^{\frac{1}{2}}} \quad \text{for } \frac{a}{c}>1. \tag{40}$$
In the case of a prolate spheroid broad-side-on and an oblate spheroid edge-on, a is equal to c and (36) reduces to
$$\frac{R_s}{a} = \frac{\frac{8}{3}\left(1-\frac{a^2}{c^2}\right)^{\frac{3}{2}}}{\left(3-2\frac{c^2}{a^2}\right)\cos^{-1}\left(\frac{c}{a}\right)-\frac{c}{a}\left(1-\frac{c^2}{a^2}\right)^{\frac{1}{2}}} \quad \text{for } \frac{c}{a}<1, \tag{41}$$
and
$$\frac{R_s}{a} = \frac{\frac{8}{3}\left(\frac{a^2}{c^2}-1\right)^{\frac{3}{2}}}{\left(2\frac{c^2}{a^2}-3\right)\cosh^{-1}\left(\frac{c}{a}\right)+\frac{c}{a}\left(\frac{c^2}{a^2}-1\right)^{\frac{1}{2}}} \quad \text{for } \frac{c}{a}>1. \tag{42}$$
Curves 1 and 2 on figure 6 were calculated from (39–40) and (41–42) respectively. Dots were obtained by the presented technique using 14 singular points distributed symmetrically near the centre of the particle at positions ($\pm 0.01, 0, 0$), ($0, \pm 0.01, 0$), $0, 0, \pm 0.01$) and ($\pm 0.05, \pm 0.05, \pm 0.05$). Surface points 66 in number have been used to define the shape of the spheroids.

As expected, the error in the calculations is small for slightly deformed spheres and grows for large elongations. However, even when the singularities were distributed near the centre of the particle the error was below 3 % for an aspect ratio of the spheroid below 2. For aspect ratios 0.7 to 1.6 the error is usually below 1 % for a wide class of distributions of the singularities. Also the number of surface points is not critical, unless they are unsymmetrically distributed.

As a last example let us consider a spheroidal particle with aspect ratio 2 : 1 : 1 freely suspended in a simple shear flow. Calculations were performed using the same number and distributions of the singularities as above. Simple shear flow in dimensionless form can be expressed as $v_x = z$, $v_y = 0$, $v_z = 0$. Initially the spheroid was oriented with its long axis in the direction of the flow, and for this orientation the translational velocity and angular velocity of the spheroid was calculated. Next, the particle was rotated by 15° with respect to the y-axis and new translational and angular velocities were calculated. This process was continued until the spheroid returned to its original

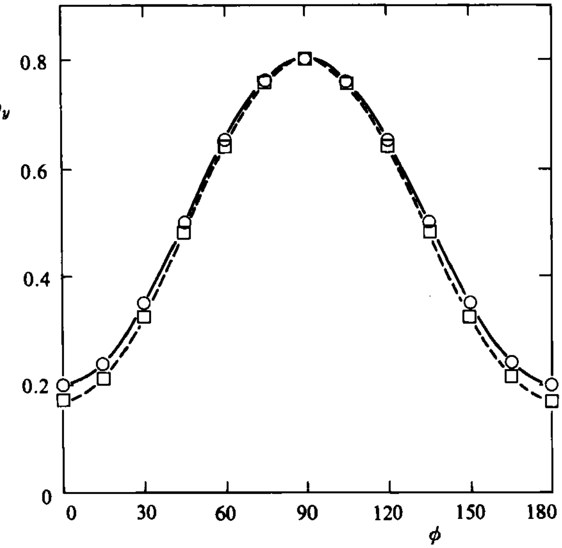

FIGURE 7. Angular velocity ω_y of a spheroidal (2:1:1) particle in a simple shear flow as a function of the orientation angle ϕ: circles and squares, particle centre–wall separation equal to 200 and 2.1 respectively.

orientation. Rotation of the body was achieved by transformation of all surface points x_s, y_s, z_s to their new positions. It was assumed that the body rotated through an angle ϕ about a line through the body centre, whose direction-angles are α, β and γ. The coordinates X_s, Y_s, and Z_s of the new position of a point whose original coordinates were (x_s, y_s, z_s) can be expressed by the equations

$$X_3 = (\xi^2-\eta^2-\zeta^2+\chi^2)\,x_s+2(\xi\eta-\zeta\chi)\,y_s+2(\xi\zeta+\eta\chi)\,z_s,$$
$$Y_3 = 2(\xi\eta+\zeta\chi)\,x_s+(-\xi^2+\eta^2-\zeta^2+\chi^2)\,y_s+2(\eta\zeta-\xi\chi)\,z_s,$$
$$Z_3 = 2(\xi\zeta-\eta\chi)\,x_s+2(\eta\zeta-\xi\chi)\,y_s+(-\xi^2-\eta^2+\zeta^2+\chi^2)\,z_s,$$

where $$\xi = \cos\alpha\,\sin(\tfrac{1}{2}\phi), \quad \zeta = \cos\gamma\,\sin(\tfrac{1}{2}\phi),$$

and $$\eta = \cos\beta\,\sin(\tfrac{1}{2}\phi), \quad \chi = \cos(\tfrac{1}{2}\phi).$$

Far away from the wall a spheroid in any angular orientation follows fluid streamlines. Its angular velocity depends on the angle between the long semi-axis and the x-axis of the coordinate system. The solid lines in figure 7 were calculated from Jeffery's (Burgers 1938) solution for the case of an ellipsoid of revolution. According to this solution the angular velocity of the particle ω_y can be expressed as

$$\omega_y = \frac{G(a^2\cos^2\phi+b^2\sin^2\phi)}{a^2+b^2}, \tag{43}$$

where G is the shear rate.

Dots in figure 7 have been calculated using the present technique. For all orientations of the spheroid, when the separation between particle and wall was large ($z > 100$), the difference between theoretical and calculated values of the angular velocity was below 1 %. The broken line in figure 7 connects the calculated values of ω_y when the distance between particle and wall equals 2.1. As one can see, for $\phi = 0°$

and 180°, i.e. when the spheroid is oriented parallel to the wall, the angular velocity is reduced. However, for perpendicular orientations the angular velocity becomes almost identical to that for infinite separation. This is the result of the strong interaction between the lower end of the spheroid and the wall, enhancing the rotation.

5. Discussion and concluding remarks

The method presented allows one to find approximate values of hydrodynamic forces and torques as well as translational and angular velocities of particles in an arbitrary external flow field. Hydrodynamic interactions with a wall can easily be taken into account. As base functions of the method, singular fundamental solutions of the Stokes equation are used for a point force and a point source in the presence of the wall on which the no-slip boundary condition is applied. Because such solutions were also found for Stokeslets between two parallel flat plates (Linon & Michon 1976*a*), the method can be easily generalized for channel flow. Stokeslets in two fluid spaces have been discussed by Aderogba (1976).

In order to calculate the hydrodynamic drag on spherical particles we have generalized Burgers' idea of looking for such values of the singular forces, located in the particle centre, that make the mean values of the velocity components vanish over the individual particle surface. A numerical procedure which allows one to perform the calculations requires only information about positions of the spheres and the external flow field. This approach gives fairly good results for systems of two or more spheres placed in a uniform flow or moving under external forces. Effects related to wall interactions can be readily studied with relatively small errors, provided that the particle–wall separation is higher than the particle diameter. In order to make the calculations more accurate for smaller separations and also to allow the calculation of the torque on the particles, we have introduced additional singularities distributed in the vicinity of the particle centre. Optimum values of the additional singular forces and sources can be found by minimizing the residual velocity in a number of surface points of each particle after introducing one singular force in a manner described earlier. It was found, however, that a one-step approach in which only the differences between the fluid and surface-element velocities are minimized, e.g. in least-square sense, leads to the same results. It appears that the least-square approximation gives reasonable results. Also the solution obtained by minimizing the L1 norm seems to give proper results, although the procedure was found not to be adequate to provide proper results in every situation. Attempts to use the Chebyshev norm were even more discouraging.

Test calculations show that using 6 or 12 singular forces and sources placed symmetrically in the vicinity of the sphere centre can give results with errors below 1 % if no relative motion of the particles at small separations is observed. If such relative movement exists, e.g. when a sphere approaches a solid plane perpendicularly, the error is small for separations larger than 20 % of the particle radii. However, it was shown that the error can be reduced to small values for even smaller separations if more singularities and more surface points are used in the calculations.

In order to obtain direct information about particle translational and angular velocities a general computational method was proposed. In this case one must specify external forces and torques acting on the particle, their shape, the external flow field and the positions of the particles. In such an approach translational and angular velocities can be calculated directly. The test calculations performed for spherical and spheroidal particles show that a direct solution by orthogonal transformations of the linearly constrained least-square problem is more efficient than the Lagrangian multiplier approach which leads to a determined system of linear equations. The accuracy in the calculations of drag forces by both methods seems to be in the same range when 14 singular points are used. For non-spherical particles it was found that, when the singularities were distributed in the vicinity of the particle centre, fairly good results were obtained if the aspect ratio of the ellipsoid of revolution was within the range 0.5–2.0.

Test calculations show that the results are fairly insensitive to the distribution of the singularities. For example, in the case of spheroids no improvement was achieved when the singularities were distributed on an ellipsoidal instead of a spherical surface situated inside the particle. However for very elongated objects, e.g. for long cylinders, better results may be expected when the singularities are distributed along the body rather than in the centre.

Finally, we wish to discuss some advantages and disadvantages of the method as compared to others which are, or could be, used to solve similar problems. The proposed technique is an approximated one and some effort is required in order to find the error in the calculations. More detailed studies of the integral representation of the solutions can indicate the optimum distribution of singularities. This could make the method more relevant for analysis of specific systems. A method widely used in numerical analysis, of gaining information about errors by repeating the calculations with different number of singular and surface points can provide sufficient insight into the accuracy of these calculations. The advantages of the method are evident. The calculations are easy to perform, relatively fast and the technique is general in the sense that it can deal with systems without symmetry; however, if symmetry exists it can be readily exploited in order to reduce the amount of computation. The presented technique can be used to calculate directly the translational and angular velocities of the individual particles. Calculations are equally easy to perform for spherical as well as for non-spherical particles, and a wide range of wall interactions can readily be taken into account.

The singularity method described in the paper can be regarded as useful alternative to other techniques especially when particle–particle and particle–wall separations are not too small. For such cases the boundary-collocation or integral-equation techniques can provide better results.

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