Integral equation methods for Stokes flow in doubly-periodic domains

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Abstract. A fast integral-equation technique is presented for the calculation of Stokes flow in doubly-periodic domains. While existing integral formulations typically rely on a Fourier series to compute the governing Greens' function, here a method of images is developed which is faster, more flexible, and easily incorporated into the fast multipole method. Accurate solutions can be obtained with obstacles of arbitrary shape at a cost roughly proportional to the number of points needed to resolve the interface. The performance of the method is illustrated with several numerical examples.

Key words: biharmonic equation, doubly-periodic, fast multipole method, integral equations, Stokes flow

1. Introduction

The study of the flow of a viscous fluid past an assemblage of particles, whether they be in a suspension or fixed as in a porous medium, is important in many physical and biological processes. On a large scale, these assemblages can be viewed as homogeneous media with some transport coefficients characterizing the microstructure. Examples include the permeability or dispersion tensors of a porous medium, and the effective viscosity or settling velocity of a suspension. Thus, it is of considerable technological importance to be able to determine these coefficients from a knowledge of the microstructure (the "forward" problem) or to extract some information about the microstructure from measured flow properties (the "inverse" problem). In both cases, numerical simulation is a desirable option, since experimentation is costly. Even with modern computational hardware, however, accurate calculations of transport properties are extremely difficult. One must compute fluid flow in highly complicated domains of sufficiently large size that the domain is a true representation of the bulk environment. This can involve thousands of independent simulations, each involving thousands of particles, in order to carry out an appropriate statistical analysis. Even then, certain simplifications are necessary. A common first step is to view the medium or suspension as composed of the periodic replication of a representative unit "cell". With periodic boundary conditions imposed, a variety of further simplifications are often made. These may include, for example, the use of regular arrays of particles of simple shape, asymptotic approximation of the underlying hydrodynamic interactions, and estimates of the properties based on low-order statistics.

The aim of this paper is to present a fast and accurate algorithm for the computation of Stokes flow past solid particles in a doubly-periodic domain, induced by an applied pressure gradient. The method extends our work presented in [1, 2] for Stokes flow in multiply-connected unbounded or wall-bounded domains. It is closely related to the work presented in

[3], which considers the analogous periodic problem in planar elasticity. The integral represent-
ations, however, are different in the two cases, as the incorporation of the pressure field at
infinity gives rise to some interesting problems in complex analysis, described in Section 3.

A number of integral-equation approaches have been suggested for solving the periodic
Stokes-flow problem. Larson and Higdon [4, 5], for example, consider simple shapes on
regular lattices. Instead of using periodic kernels in the integral representation, they enforce
the boundary conditions by discretizing the perimeter of the unit cell and imposing periodic
boundary conditions there. Zick and Homsy [6] and Tran-Cong *et al.* [7] use fundamental
solutions which explicitly take into account periodicity. While they do not have to discretize
the cell boundary, their integral equation is of the first kind and can suffer from ill-conditioning
when fine discretization is used. Drummond and Tahir [8] describe a complex-variable method
for regular arrays of cylinders. Their approach is related to ours in the treatment of period-
icity, but is not applicable to particles of arbitrary shape. Other recent work includes van de
Vorst's viscous-sintering calculations [9, 10] and the work on suspensions by Li, Charles and
Pozrikidis [11–14], and Fan *et al.* [15]. In all these approaches, a number of distinct issues
arise. These include the computation of the Green's function, the choice of direct *vs.* iterative
method, and the incorporation of a fast algorithm, if desired. Classical direct methods, of
course, require $O(N^3)$ work. With a well-conditioned integral equation, iterative methods
require $O(N^2)$ work. A variety of fast algorithms can be incorporated to reduce the cost to
$O(N)$ or $O(N \log N)$, as discussed below.

A different approach to carrying out large-scale simulations makes use of simplifying
approximations of the underlying hydrodynamical model. This includes the "Stokesian dy-
namics" approach of Brady *et al.* [16–18], or Sangani and Mo [19]. In essence, details of
the hydrodynamic interactions are neglected, and particles interact according to an assembled
"mobility matrix". While lubrication effects can be incorporated into the model, the approach
is most reliable for dilute arrays of simple particle shape.

Finally, there have been a number of studies using finite-difference or finite-element meth-
ods [20–23], mostly in the context of low-Reynolds-number calculations. These have gener-
ally been limited to small-scale examples.

In order to develop an approach that is both fast and applicable to obstacles of arbi-
trary shape, we derive a simple integral representation for the flow field using the classical
complex-variable theory for the biharmonic equation. Discretization of the corresponding
integral equation leads to a dense linear system of equations, which is solved iteratively with
fast multipole acceleration [24–27] to compute the matrix-vector products. With N points in
the discretization of the boundary, our method requires only $O(N)$ operations. Thus one can
solve large-scale problems with only modest computational resources.

For a good overview of integral-equation methods in Stokes flow, we refer the reader to
the texts [28, 29]. For a discussion of the relation between the primitive-variable techniques
employed there with the complex-variable formulation described here, see [1]. Recent work
by Gomez and Power, similar in spirit to that presented here, can be found in [30].

The main contribution of the present work is contained in Section 3, where a new technique
is discussed for the computation of conditionally convergent lattice sums. Specifically, we are
able to impose periodicity on the fluid quantities together with a pressure gradient across a unit
cell, and we are also able to incorporate these lattice sums easily into a fast multipole-based
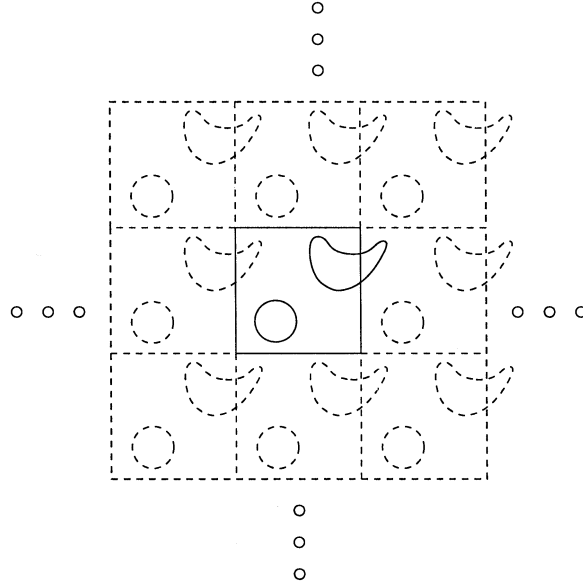framework.

Figure 1. A square unit cell with two obstacles and its eight nearest neighbours. The image cells extend in all directions. Note that one of the obstacles intersects the cell boundary.

2. The biharmonic potential and the Sherman-Lauricella representation

We consider slow viscous flow in a medium containing an infinite collection of solid particles. The medium consists of the periodic extension of a representative unit cell and, to simplify the ensuing discussion, we assume the unit cell is the square $D_0 = [-1/2, 1/2] \times [-1/2, 1/2]$ (Figure 1). Given M obstacles per unit cell ($D_1, \cdots, D_M$) with boundaries ($\Gamma_1, \cdots, \Gamma_M$), we denote the area fraction they occupy by c, and the union of all obstacles boundaries by Γ. The governing equations in the fluid domain $D = D_0 - D_1 - \cdots - D_M$, are the linear Stokes equations

$$\mu \Delta u = \frac{\partial p}{\partial x}, \qquad \mu \Delta v = \frac{\partial p}{\partial y} \tag{1}$$

$$u_x + v_y = 0, \tag{2}$$

where u and v are the x and y components of velocity respectively, μ is the viscosity, and p is the pressure. An additional physical quantity of interest is the vorticity

$$\zeta = -u_y + v_x.$$

We restrict our attention to problems where the particles are fixed. Thus, on the boundary, no-slip conditions are satisfied

$$u = 0, \qquad v = 0, \qquad \text{for } \mathbf{t} \in \Gamma . \tag{3}$$

The governing equations can be simplified by introducing a stream function $W(x, y)$ defined by

$$u = \frac{\partial W}{\partial y}, \qquad v = -\frac{\partial W}{\partial x}, \qquad \zeta = -\Delta W.$$

In this way, (2) is automatically satisfied, and (1), together with the boundary conditions (3), yields

$$\Delta^2 W(\mathbf{x}) = 0, \qquad \text{for } \mathbf{x} \in D,$$
$$\nabla W = 0, \qquad \text{for } \mathbf{t} \in \Gamma. \tag{4}$$

Following the discussion of Mikhlin and others [31–33], we note that any plane biharmonic function $W(x, y)$ can be expressed by Goursat's formula as

$$W(x, y) = \mathfrak{Re}(\overline{z}\phi(z) + \chi(z)),$$

where ϕ and χ are analytic functions of the complex variable $z = x + \mathrm{i}y$, and $\mathfrak{Re}(f)$ denotes the real part of the complex function f. The functions $\phi(z)$ and $\psi(z) = \chi'(z)$ are known as the Goursat functions. A simple calculation leads to Muskhelishvili's formula

$$\frac{\partial W}{\partial x} + \mathrm{i}\frac{\partial W}{\partial y} = \phi(z) + z\overline{\phi'(z)} + \overline{\psi(z)}, \tag{5}$$

providing us with an expression for the velocity in Stokes flow. The pressure and vorticity can be expressed in terms of the Goursat functions, as

$$\zeta + \frac{\mathrm{i}}{\mu} p = -4\phi'(z). \tag{6}$$

Muskhelishvili's formula (5) allows us to formulate the problem in the context of analytic-function theory and seek the functions ϕ and ψ which satisfy appropriate conditions on the boundary Γ. These conditions are

$$\phi(t) + t\overline{\phi'(t)} + \overline{\psi(t)} = 0, \tag{7}$$

for $t \in \Gamma$. Here, we have identified the point $\mathbf{t} \in \mathbf{R}^2$ with the complex point $t \in \mathbf{C}$.

Suppose first that D_0 is the entire plane, so that the fluid domain D is unbounded. To find the analytic functions $\phi(z)$ and $\psi(z)$ that satisfy the boundary conditions (3), we start with the representations established in [1]:

$$\phi(z) = \frac{1}{2\pi\mathrm{i}} \int_\Gamma \frac{\omega(\xi)}{\xi - z} \, \mathrm{d}\xi + \int_\Gamma \omega(\xi) \, \mathrm{d}s + \sum_{k=1}^{M} C_k \log(z - z_k), \tag{8}$$

$$\psi(z) = \frac{1}{2\pi\mathrm{i}} \int_\Gamma \frac{\overline{\omega(\xi)} \, \mathrm{d}\xi + \omega(\xi) \, \mathrm{d}\overline{\xi}}{\xi - z} - \frac{1}{2\pi\mathrm{i}} \int_\Gamma \frac{\overline{\xi}\omega(\xi)}{(\xi - z)^2} \, \mathrm{d}\xi + \sum_{k=1}^{M} \frac{b_k}{z - z_k}$$

$$+ \sum_{k=1}^{M} \overline{C}_k \log(z - z_k) - \sum_{k=1}^{M} C_k \frac{\overline{z}_k}{z - z_k}. \tag{9}$$

In the preceding expressions, $\omega(\xi)$ is an unknown complex density, z_k are arbitrarily prescribed points inside the component curves Γ_k, and $\mathrm{d}s$ is an element of arc length. It is important to observe that while ϕ and ψ are not single-valued functions, the physical variables of interest (velocity, pressure, and vorticity) are well-defined. It is also important to note that while some terms in the Goursat functions are not independent of the coordinate system, the

physical quantities are. The complex velocity field is given by

$$-v + \mathrm{i}u = \frac{\partial W}{\partial x} + \mathrm{i}\frac{\partial W}{\partial y} = \frac{1}{2\pi\mathrm{i}} \int_\Gamma \frac{\omega(\xi)}{\xi - z}\,\mathrm{d}\xi + \int_\Gamma \omega(\xi)\,\mathrm{d}s - \frac{1}{2\pi\mathrm{i}} \int_\Gamma \frac{\overline{\omega(\xi)}\,\mathrm{d}\xi + \omega(\xi)\,\mathrm{d}\overline{\xi}}{\overline{\xi} - z}$$

$$+ \frac{1}{2\pi\mathrm{i}} \int_\Gamma \frac{(\xi - z)\overline{\omega(\xi)}}{(\overline{\xi} - z)^2}\,\mathrm{d}\overline{\xi} + \sum_{k=1}^{M} \frac{\overline{b_k}}{(\overline{z} - \overline{z}_k)} + \sum_{k=1}^{M} 2C_k \log\|z - z_k\| + \sum_{k=1}^{M} \overline{C_k}\frac{z - z_k}{\overline{z - z_k}}. \quad (10)$$

To establish a connection with singularities expressed in primitive variables, we note that the terms involving b_k and C_k are "Rotlets" and "Stokeslets", respectively. A more detailed discussion of their role in the integral-equation formulation can be found in [1]. Physically, these singularities correspond to the hydrodynamic torque and force acting on the solid particle (*c.f.* [2]). In order to ensure that the flow is bounded at infinity, it is sufficient to require that

$$\sum_{k=1}^{M} C_k = 0, \tag{11}$$

and we refer to the sum of the left-hand side of (11) as the *net Stokeslet moment.*

3. Periodic boundary conditions

There are a number of ways of imposing periodic boundary conditions. In the simplest approach, one can work with the free-space Green's function, discretize the perimeter of the unit square, and impose periodicity explicitly. However, there are two obvious objections to this approach. First, it increases the number of degrees of freedom and complicates the linear system needed to be solved. Second, it is inconvenient in dealing with obstacles *intersecting* the unit square (Figure 1). The alternative, namely to work with an appropriately defined Green's function, carries its own burden. One must develop an effective procedure for its evaluation. One popular approach is to compute the Green's function in terms of Fourier series [34] using the acceleration technique pioneered by Ewald [35]. An alternative is the method of images, introduced by Lord Rayleigh [36], which has been extended to the case of Stokes flow in an interesting series of papers [8, 37, 38]. The latter approach has a number of advantages in terms of speed, as it allows for the precomputation of certain lattice sums in terms of which the Green's function can be rapidly obtained. Moreover, it is easy to incorporate into the fast multipole method (FMM). Nevertheless, it has only been used, to the authors' knowledge, in considering regular arrays of cylinders (or spheres in the three-dimensional case). Perhaps one of the impediments to its application and widespread use is the difficulty of dealing with a modest number of divergent and conditionally convergent series.

In this section, we give a fairly comprehensive description of a method of images based on the complex-variable formulation of Stokes flow presented in Section 2. This is similar in many respects to that developed by Drummond and Tahir [8] and the discussion of plane elasticity in [3]. To begin, let $\mathbf{Z}^2$ denote the set of lattice points in the plane with integer coordinates,

$$\mathbf{Z}^2 = \{k_1 + \mathrm{i}k_2 \mid k_1, k_2 \in \mathbf{Z}\},$$

and let Λ denote the punctured lattice

$$\Lambda = \{k_1 + \mathrm{i}k_2 \mid k_1, k_2 \in \mathbf{Z}, k_1^2 + k_2^2 \neq 0\}.$$

We proceed by replacing the kernels of the integral operators in (10) by their periodic analogs. Thus, instead of the Cauchy kernel $1/(\xi - z)$, we use the Weierstrass ζ function

$$\zeta(\xi - z) = \sum_{w \in \mathbf{Z}^2} \frac{1}{w + \xi - z}, \tag{12}$$

and instead of the kernel $(\xi - z)/(\bar{\xi} - \bar{z})^2$, we use the function

$$\eta(\xi - z) = \sum_{w \in \mathbf{Z}^2} \frac{w + \xi - z}{(\bar{w} + \bar{\xi} - \bar{z})^2}. \tag{13}$$

The periodic extension of the discrete source terms in Equation (10) requires consideration of the functions

$$\mathcal{S}(\xi - z) = \sum_{w \in \mathbf{Z}^2} \log(w + \xi - z), \tag{14}$$

$$\mathcal{D}(\xi - z) = \sum_{w \in \mathbf{Z}^2} \frac{w + \xi - z}{\bar{w} + \bar{\xi} - \bar{z}} \tag{15}$$

as well. Thus, we seek to define a *periodic* velocity field in terms of the representation

$$\begin{aligned}
-v + \mathrm{i}u = {} & \frac{\partial W}{\partial x} + \mathrm{i}\frac{\partial W}{\partial y} = \frac{1}{2\pi\mathrm{i}} \int_\Gamma \omega(\xi)\zeta(\xi - z)\,\mathrm{d}\xi + \int_\Gamma \omega(\xi)\,\mathrm{d}s \\
& - \frac{1}{2\pi\mathrm{i}} \int_\Gamma \overline{\zeta(\xi - z)}\,[\overline{\omega(\xi)}\,\mathrm{d}\xi + \omega(\xi)\,\mathrm{d}\bar{\xi}] + \frac{1}{2\pi\mathrm{i}} \int_\Gamma \overline{\omega(\xi)}\,\eta(\xi - z)\,\mathrm{d}\bar{\xi} \\
& + \sum_{k=1}^M \overline{b_k}\,\overline{\zeta(z_k - z)} + \sum_{k=1}^M 2\,C_k\,\Re\,(\mathcal{S}(z_k - z)) + \sum_{k=1}^M \overline{C_k}\,\mathcal{D}(z_k - z). \tag{16}
\end{aligned}$$

Care must be taken in working with the functions $\zeta(\xi - z)$, $\eta(\xi - z)$, $\mathcal{S}(\xi - z)$, and $\mathcal{D}(\xi - z)$ since the series (12), (13), (14), and (15) are either conditionally convergent or divergent. To develop appropriate values for these functions, we use a Taylor expansion for each value w in the punctured lattice Λ:

$$\zeta(\xi - z) = \frac{1}{\xi - z} + \left[\sum_{w \in \Lambda} \frac{1}{w}\right] - (\xi - z)\left[\sum_{w \in \Lambda} \frac{1}{w^2}\right] + (\xi - z)^2 \left[\sum_{w \in \Lambda} \frac{1}{w^3}\right] - \dots, \tag{17}$$

$$\begin{aligned}
\eta(\xi - z) = {} & \frac{\xi - z}{(\bar{\xi} - \bar{z})^2} + \left[\sum_{w \in \Lambda} \frac{w}{\bar{w}^2}\right] - 2(\bar{\xi} - \bar{z})\left[\sum_{w \in \Lambda} \frac{w}{\bar{w}^3}\right] + 3(\bar{\xi} - \bar{z})^2\left[\sum_{w \in \Lambda} \frac{w}{\bar{w}^4}\right] - \dots \\
& - (\xi - z)\left[\sum_{w \in \Lambda} \frac{1}{\bar{w}^2}\right] + 2(\xi - z)(\bar{\xi} - \bar{z})\left[\sum_{w \in \Lambda} \frac{1}{\bar{w}^3}\right] \\
& - 3(\xi - z)(\bar{\xi} - \bar{z})^2\left[\sum_{w \in \Lambda} \frac{1}{\bar{w}^4}\right] + \dots, \tag{18}
\end{aligned}$$

$$\mathcal{D}(\xi - z) = \frac{\xi - z}{\bar{\xi} - \bar{z}} + \left[\sum_{w \in \Lambda} \frac{w}{\bar{w}}\right] - (\bar{\xi} - \bar{z}) \left[\sum_{w \in \Lambda} \frac{w}{\bar{w}^2}\right] + (\bar{\xi} - \bar{z})^2 \left[\sum_{w \in \Lambda} \frac{w}{\bar{w}^3}\right] - \ldots$$

$$- (\xi - z) \left[\sum_{w \in \Lambda} \frac{1}{\bar{w}}\right] + (\xi - z)(\bar{\xi} - \bar{z}) \left[\sum_{w \in \Lambda} \frac{1}{\bar{w}^2}\right] \tag{19}$$

$$- (\xi - z)(\bar{\xi} - \bar{z})^2 \left[\sum_{w \in \Lambda} \frac{1}{\bar{w}^3}\right] - \ldots,$$

and

$$\mathcal{S}(\xi - z) = \log(\xi - z) + \left[\sum_{w \in \Lambda} \log w\right] + (\xi - z) \left[\sum_{w \in \Lambda} \frac{1}{w}\right]$$

$$- \frac{(\xi - z)^2}{2} \left[\sum_{w \in \Lambda} \frac{1}{w^2}\right] + \ldots. \tag{20}$$

The lattice sums in these expressions are generally denoted by

$$S_j = \sum_{w \in \Lambda} \frac{1}{w^j}, \qquad j \geq 1,$$

and

$$T_j = \sum_{w \in \Lambda} \frac{w}{\bar{w}^{j-1}}, \qquad j \geq 2.$$

For consistency, we define

$$S_0 = \sum_{w \in \Lambda} \log w.$$

Note that the sums S_j, for $j \geq 3$, and T_j, for $j \geq 5$, are convergent. Note also that S_0, S_1, T_2 and T_3 are the constant terms in the expansions (17–20). It is straightforward to show that setting them all to zero preserves periodicity. The conditionally convergent sums S_2 and T_4 are a little more subtle, with values dependent on the geometry of the lattice Λ. If we require that ζ, η and $\mathcal{D}$ be doubly periodic on the unit square, it can be shown [8, 3, 36] that S_2 should be set to π, while T_4 is approximately $4 \cdot 07845116116140$.

It remains only to consider the imposition of a pressure gradient, which has an interesting interpretation in terms of complex variable theory. Recall from (6) that $\phi'(z)$ satisfies

$$\zeta + \frac{i}{\mu} p = -4\phi'(z).$$

Thus, we seek Goursat functions $\phi(z)$ and $\psi(z)$ for which the vorticity $\zeta = -4\Re[\phi'(z)]$ and the velocity field $\phi(z) + z\overline{\phi'(z)} + \overline{\psi(z)}$ are periodic on the unit cell, but for which the pressure $p = -4\mu\Im[\phi'(z)]$ satisfies either

$$p(x + 1/2, y) = p(x - 1/2, y) - 1, \qquad p(x, y + 1/2) = p(x, y - 1/2), \tag{21}$$

or

$$p(x + 1/2, y) = p(x - 1/2, y), \qquad p(x, y + 1/2) = p(x, y - 1/2) - 1. \tag{22}$$

The first case corresponds to an applied pressure gradient in the x-direction and the second case to an applied pressure gradient in the y-direction. The effective permeability tensor $\mathcal{K}$ is defined by the linear relation

$$\left\langle \begin{matrix} v_1 \\ v_2 \end{matrix} \right\rangle = \mathcal{K} <\nabla p>,$$

where $<v_1, v_2>^T$ is the average velocity field over the fluid domain in the periodic cell and $<\nabla p>$ is the average pressure gradient. Thus, by evaluating the velocity field under the conditions (21), we obtain the tensor components K_{11} and K_{21}. Evaluating the velocity field under the conditions (22) yields K_{21} and K_{22}.

We are able to establish the desired boundary conditions by means of the following result.

LEMMA 3.1. *Suppose that*

$$\phi(z) = \frac{1}{2\pi i} \int_\Gamma \omega(\xi)\zeta(\xi - z)\,d\xi + \int_\Gamma \omega(\xi)\,ds + \sum_{k=1}^M C_k\, \mathcal{S}(z_k - z), \tag{23}$$

and that the corresponding velocity field is given by (16) with the non-convergent lattice sums defined as above. If the net Stokeslet moment $\sum_{k=1}^M C_k$ equals $i/2\pi$, then the velocity field is periodic, while the pressure satisfies (21). Similarly, if $\sum_{k=1}^M C_k = 1/2\pi$, then the velocity field is periodic, while the pressure satisfies (22).

Sketch of proof: Although the details are somewhat involved, the essence of the idea is simple. First, if there is no net Stokeslet moment in the unit cell ($\sum_{k=1}^M C_k = 0$), then all physical quantities are easily shown to be periodic. Suppose now that the unit cell does support some net Stokeslet moment. Since the governing equation is linear, we can place a single Stokeslet at the origin to cancel this moment. The total field then maintains periodicity in all physical quantities. Thus, we need only consider the case of a single source at the origin. An explicit computation yields the desired result.   ∎

4.   Numerical methods

The reason for choosing the representation (16) for the velocity field is that it gives rise to a particularly attractive integral equation. By taking the limit as $x + iy = z \to t \in \Gamma$, and using the standard jump conditions for Cauchy integrals, we obtain

$$\begin{aligned}
\omega(t) &+ \int_\Gamma \omega(\xi)\,ds + \frac{1}{2\pi i}\int_\Gamma \omega(\xi)\left[\zeta(\xi - t)\,d\xi - \zeta(\bar{\xi} - \bar{t})\,d\bar{\xi}\right] \\
&- \frac{1}{2\pi i}\int_\Gamma \overline{\omega(\xi)}\left[\eta(\xi - t)d\bar{\xi} - \zeta(\bar{\xi} - \bar{t})\,d\xi\right] \\
&+ \sum_{k=1}^M 2C_k\Re\left(\mathcal{S}(z_k - t)\right) + \sum_{k=1}^M \overline{C}_k\mathcal{D}(z_k - t) + \sum_{k=1}^M \overline{b_k}\zeta(z_k - t) = 0.
\end{aligned} \tag{24}$$

The complex constants C_k can be defined in terms of $\omega(\xi)$ by

$$C_k = \int_{\Gamma_k} \omega(\xi)\,ds\,, \qquad \text{for } k = 2, \cdots, M, \tag{25}$$

where C_1 is fixed by the value of the pressure drop across the unit cell. As shown in the preceding section, if

$$C_1 = \frac{\mathrm{i}}{2\pi} - \sum_{k=2}^{M} C_k, \tag{26}$$

then the average pressure gradient is of unit magnitude in the x-direction. The constants b_k are real and may be defined by

$$b_k = \mathrm{i} \int_{\Gamma_k} \omega(t)\mathrm{d}\bar{t} - \overline{\omega(t)}\mathrm{d}t. \tag{27}$$

A simple calculation shows that a remarkable cancellation of singularities has occurred. Equation (24) is a second kind Fredholm equation with a *smooth* kernel, derived for a singly connected interior domain by Sherman and Lauricella [31–33]. In the absence of a spurious resonance, such equations have bounded condition number independent of the number of points used in the discretization and are ideally suited for iterative methods. For a discussion of invertibility, see [32, 33].

We now consider the discretization of our integral equation. In the present work, we use a simple quadrature based on the trapezoidal rule. If distinct portions of the interface Γ are well separated, then this approach achieves spectral accuracy for smooth data on smooth, closed contours. As a rule of thumb, collocation points on nonadjacent portions of the boundary should be at least $5h - 10h$ away, where h is the spacing of the discretization points. If, however, the obstacles are close to touching or the boundary of an obstacle folds back onto itself, then the integrand may not appear smooth even though the density ω is well resolved. In these cases, specialized quadrature is required [3].

Here, we are primarily interested in the analytic formulation of the problem, and assume that we are given N_k points on each contour Γ_k, equispaced with respect to some parametrization $t^k : [0, L_k] \rightarrow \Gamma_k$. Associated with each such point, denoted by t_j^k, is an unknown value ω_j^k. The derivative $(t^k)'$ will be denoted by σ^k, and the derivative values σ_j^k at the discretization points will be assumed or given. The step length in the discretization is defined by $h_k = L_k/N_k$, and the total number of points is

$$N = \sum_{k=1}^{M} N_k.$$

The integral equation (24) is then replaced by a discrete linear system in a straightforward manner from the trapezoidal approximation of the corresponding integrals, including those in (25) and (27). Some care must be taken, however, in evaluating the diagonal terms, as the kernels of the integral operators in (24) need to be replaced by the appropriate limits, which involve the curvature at the collocation point. If the curvature is not given, the smooth kernels

$$[\zeta(\xi - t)\,\mathrm{d}\xi - \zeta(\bar{\xi} - \bar{t})\,\mathrm{d}\bar{\xi}] \qquad \text{and} \qquad [\eta(\xi - t)\mathrm{d}\bar{\xi} - \zeta(\bar{\xi} - \bar{t})\,\mathrm{d}\xi]$$

can be interpolated to high-order accuracy without difficulty.

Remark 4.1.   We refer to the system of equations (24)–(27) as the *unconstrained* formulation.

Remark 4.2.   For the purposes of iterative solution, it is sometimes convenient to separate out the influence of the source terms involving the constants C_k. One can then discretize Equation

(24), considering the constants C_k as unknown. To compensate for the increase in system size, we add $M - 1$ constraints of the form

$$\int_{\Gamma_k} \omega(\xi)\, \mathrm{d}s = 0 \,, \qquad \text{for } k = 2, \cdots, M. \tag{28}$$

Equation (25) is no longer used, but the relations (26) and (27) are kept. We refer to the system (24), (26)–(28) as the *constrained* formulation. When solving this system iteratively, one can use the Equations (26)–(28) as a preconditioner coupled with a version of (24) from which the integral operators have been omitted:

$$\omega(t) + \sum_{k=1}^{M} 2C_k \Re\left(\mathcal{S}(z_k - t)\right) + \sum_{k=1}^{M} \overline{C}_k \mathcal{D}(z_k - t) + \sum_{k=1}^{M} \overline{b_k} \zeta(z_k - t) = 0 \,. \tag{29}$$

The cost of inverting the preconditioner is clearly of the order $O(M^3)$ since it is a rank M perturbation of the identity. The *constrained* formulation can, of course, be used with or without preconditioning.

4.1. FAST MULTIPOLE ACCELERATION

Discretization of (24) or its periodic counterpart results in a dense linear system, for which $O(N^2)$ work is required to generate the matrix. Note, however, that different schemes for evaluating the matrix entries can have noticeable impact on performance. When the number of unknowns is sufficiently small, direct elimination can be used to solve these systems with a cost proportional to N^3. Since the linear systems are well-conditioned, conjugate-gradient-type methods such as GMRES [39] require the evaluation of a fixed number of matrix-vector products which depends on the error tolerance and the geometry of the particular example but not on N. Thus, appropriate iterative techniques require $O(N^2)$ work. In order to reduce the amount of work to $O(N)$, we make use of the fast multipole method or FMM [24–26], which is a "matrix-free" approach. We refer the reader to this literature for a description of the method and to [3, 1] for its use in related problems. The incorporation of periodic boundary conditions into fast multipole methods is discussed in some detail in [40, 25].

5. Numerical results

The algorithms described in Section 3 have been implemented in Fortran. Here, we illustrate the performance on a variety of examples.

Example 1. (Regular array of disks): We consider the steady motion of a viscous fluid through a regular square array of cylinders with radius r, corresponding to an area fraction or "solid concentration" of $c = \pi r^2$. To compare with previous numerical and analytical results, we compute the dimensionless drag on the cylinder, $D = F/\mu U$, where U is the computed average velocity through the unit cell, and F is found by [2]

$$F = -8\pi \mathrm{i} C_1 \,.$$

We take $C_1 = 0{\cdot}005/\pi \mathrm{i}$, thus $F = 0{\cdot}04$. We compare with three results: the numerical results of Sangani and Acrivos [41], their asymptotic formula for the high-density case

$$D_{\text{den}} \sim \frac{9\pi}{2\sqrt{2}} \left\{ 1 - \left(\frac{c}{c_{\text{max}}}\right)^{1/2} \right\}^{-5/2} \,, \qquad c_{\text{max}} - c \ll 1$$

Table 1. Dimensionless drag $D = F/\mu U$ for various values of the solid concentration $c = \pi r^2$. The second column indicates the number of points in the discretization of the boundary, the third column indicated the number of GMRES iterations needed for the "unconstrained" integral equation, and the fourth column indicates the amount of CPU time required on a 200MHz Sun Ultra 1. The last four columns list the results of our calculations, the numerical results of Sangani and Acrivos, the dilute asymptotic approximation and the dense asymptotic approximation, respectively.

c	N	# Iterations	CPU sec	D_{calc}	$D_{\text{S\&A}}$	D_{dil}	D_{den}
0·05	64	5	0·59	15·5578	15·56	15·5578	—
0·10	64	6	0·69	24·8317	24·83	24·8323	—
0·20	64	7	0·75	51·5269	51·53	51·6068	—
0·30	64	9	0·93	102·881	102·90	105·234	—
0·40	64	10	1·03	217·894	217·89	270·011	—
0·50	64	11	1·08	$5·32548 \times 10^2$	$5·325 \times 10^2$	—	$5·44313 \times 10^3$
0·60	128	14	2·29	$1·76357 \times 10^3$	$1·763 \times 10^3$	—	$1·77523 \times 10^3$
0·70	256	19	6·15	$1·35193 \times 10^4$	$1·352 \times 10^4$	—	$1·35123 \times 10^4$
0·75	1024	26	28·68	$1·27543 \times 10^5$	$1·263 \times 10^5$	—	$1·27424 \times 10^5$
0·76	1024	30	34·05	$2·94878 \times 10^5$	—	—	$2·94615 \times 10^5$
0·77	2048	36	78·76	$1·03903 \times 10^6$	—	—	$1·03778 \times 10^6$

(here $c_{\text{max}} = \pi/4$), and the asymptotic formula for the dilute case from [8],

$$D_{\text{dil}} \sim \frac{8\pi}{\log(1/c) - 1·47633597 + 2c - 1·77428264c^2 + 4·07770444c^3 - 4·84227402c^4 + O(c^5)}.$$

A summary of the relevant data can be found in Table 1.

Example 2. (Irregular array of disks): We consider the flow past an irregular arrangement of seven disks. In Figure 2, we plot contours of the magnitude of the velocity field, pressure field and vorticity.

These results were obtained with 64 points on the boundary of each particle, resulting in a complex linear system of dimension 448. While Gaussian elimination would clearly be an appropriate solver for such a small system, we again use GMRES to study the performance of two iterative schemes (the "preconditioned" formulation of the last section and the "unconstrained" formulation). In Figure 3, we plot the residual as a function of the iteration count, where the GMRES tolerance was set to 10^{-9} and the FMM tolerance was set to 10^{-10}. The solution of the integral equation was deduced to have at least eight digits of accuracy.

Example 3. (Irregular array of irregular obstacles): We consider the flow past an irregular dispersion of eight obstacles. In Figure 4, we plot contours of the pressure and vorticity fields.

These results were obtained with 500 points on the boundary of each particle, resulting in a complex linear system of dimension 4000. This system is sufficiently large that an FMM-accelerated iterative solver is quite expedient: GMRES required 58 iterations using the preconditioned integral equation to obtain six digits of accuracy, verified by doubling the number of points, and consumes less than seven minutes of CPU time on a 440 MHz SUN Ultra10 workstation.
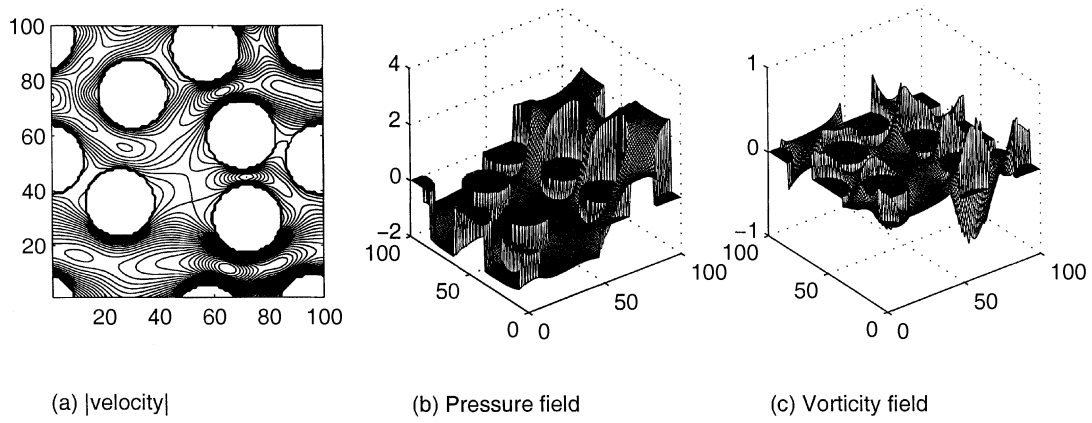
(a) |velocity| (b) Pressure field   (c) Vorticity field

Figure 2. The upper left-hand figure shows the disk placement, and the upper right-hand figure shows a contour plot of the velocity magnitude. The lower plots show the pressure and vorticity fields.
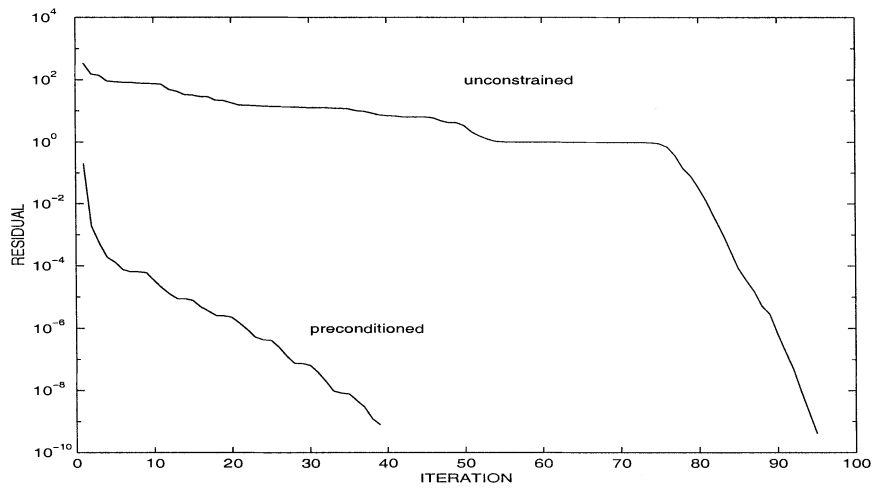

Figure 3. Performance of GMRES using the unconstrained and preconditioned integral equations in Example 2.
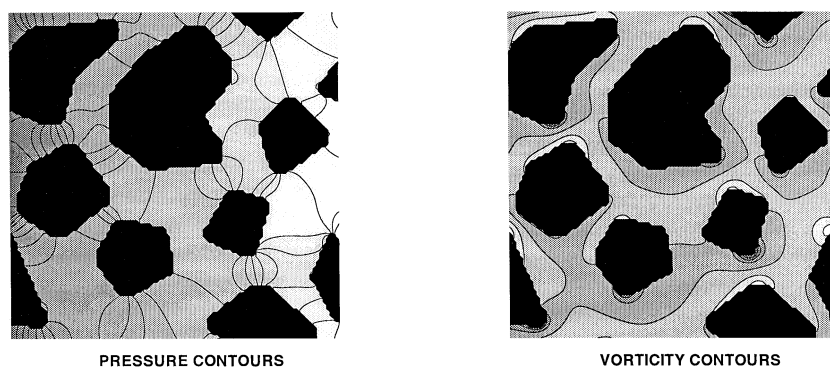

PRESSURE CONTOURS   VORTICITY CONTOURS

Figure 4. Contour plots of the pressure and vorticity fields for Example 3.

6. Conclusions

We have presented a new integral-equation method for the simulation of Stokes flow in two-dimensional doubly periodic domains. The method is spectrally accurate and, with fast multipole acceleration, requires $O(N)$ operations where N is the number of nodes in the discretization of the boundary. In order to impose a pressure gradient across the unit cell, we have incorporated a novel method of images (Section 3), which is easily incorporated into fast multipole (FMM) accelerated algorithms. The implementation has not been highly optimized. Improvement in the FMM routine and the incorporation of adaptive quadrature will result in a more effective code for large scale simulation.

We are considering the extension of our approach to three-dimensional problems. Clearly, the complex formulation does not extend to three dimensions and we will then move to a primitive variable formulation. The relevant potential theory can be found in several sources [28, 42, 29]. We also note that the computational tools are available in three dimensions [43, 44].

Acknowledgements

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