

Locally Corrected Semi-Lagrangian Methods for Stokes Flow with Moving Elastic Interfaces

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Abstract

Key words:

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1 Introduction

??John please read carefully and see what you want to modify

We present a numerical method for computing time-dependent Stokes flow in two dimensions with a moving interface consisting of material which responds elastically to its stretching. The resulting force creates jumps in the fluid velocity gradient and pressure at the interface. The Immersed Boundary Method of C. Peskin [19] has been used extensively to model biological problems with Stokes or Navier-Stokes flow with elastic interfaces. The present work develops an alternative approach for this class of problems. To move the interface we use the semi-Lagrangian contouring method developed in a series of papers [24–28]: Given the location of the curve and the fluid velocity at the current

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time, the signed distance function for the curve is found on a tree of cells and transported by the semi-Lagrangian or backward characteristic method. The curve at the new time is then contoured from this transported distance function. The fluid velocity, determined by the interface location and jump conditions, is computed as a potential integral in a periodic box using Ewald summation, with the velocity split into two parts. The smooth part is calculated as a Fourier series, while the local part is approximated using asymptotic analysis, resulting in a local correction. The velocity can be evaluated accurately at arbitrary points. The stretching of the interface, which determines the elastic force, is expressed in a simple way in terms of the computed motion of the curve. We report results for a test problem with an exact solution with time-periodic motion in which the interface is an ellipse of varying eccentricity. Our tests verify that the method is second order accurate.

We begin with the statement of the problem. We consider fluid flow in a two-dimensional periodic box modeled by Stokes flow, that is, very viscous, incompressible flow in which the material derivative in the Navier-Stokes equations is omitted. The velocity $v(x, t)$ and pressure $p(x, t)$ satisfy the equations

$$-\nu\Delta v + \nabla p = F, \quad \nabla \cdot v = 0 \quad (1.1)$$

with a force F consisting of an interfacial force on a curve Γ and possibly a body force,

$$F = f\delta_\Gamma + F_b. \quad (1.2)$$

Γ is a closed curve consisting of elastic material immersed in the fluid and moving with the fluid velocity. The interfacial force is defined by its action on a test function $w(x)$,

$$\int \int f(x)\delta_\Gamma(x)s(x) d^2x = \int_\Gamma f(x)w(x) ds(x) \quad (1.3)$$

where s is the arclength on the curve at the current time. We assume density $\rho = 1$ for simplicity.

The force term $\delta_\Gamma f$ amounts to a jump in the normal stress at the boundary (see [20]),

$$[T_{ij}]n_j = -f_i, \quad i = 1, 2 \quad (1.4)$$

with sum over j implicit, where T_{ij} is the stress tensor

$$T_{ij} = -p\delta_{ij} + \nu(v_{i,j} + v_{j,i}). \quad (1.5)$$

Here $[\cdot]$ is the outside value minus the inside, and the normal vector n points outward. Resolving this jump in normal and tangential directions, we obtain jump conditions for p and $\partial v/\partial n$ (see [20,16,17])

$$[p] = f \cdot n, \quad \nu \left[\frac{\partial v}{\partial n} \right] = -(f \cdot \tau)\tau. \quad (1.6)$$

(We assume the viscosity ν is constant.) We suppose the force f at the curve is determined by interfacial tension and thus has the form

$$f = \frac{\partial}{\partial s}(\gamma\tau) \quad (1.7)$$

where γ is the (variable) coefficient of surface tension and s is the arclength. (For derivation from classical force balance arguments, see e.g. [14,12,22]). An equivalent form of (1.7) is

$$f = (\partial\gamma/\partial s)\tau - \gamma\kappa n \quad (1.8)$$

where κ is the curvature, defined by $\partial\tau/\partial s = -\kappa n$. We assume that the interfacial tension comes from the elastic response of the material on the curve to stretching, so that γ is a function of the form

$$\gamma = \gamma(s_\alpha - 1). \quad (1.9)$$

Here α is a material coordinate, taken to be the arclength parameter in the equilibrium configuration; if the curve is parametrized as $x = X(\alpha, t)$, then

$$s_\alpha = \partial s / \partial \alpha = |\partial X / \partial \alpha|. \quad (1.10)$$

In our examples we suppose γ is linear when the stretching is positive:

$$\gamma = \gamma_0(s_\alpha - 1)^+. \quad (1.11)$$

Our formulation is the same as that of Peskin et al., except that our α corresponds to their s , and our f differs from theirs by the factor s_α . Stokes flow is an appropriate model at small scales, with viscous forces dominant, and is often used for biological problems (e.g. see references in [19]). We have included the body force F_b primarily to allow us to work with exact test problems, as was done in [17].

In Sec. 2 we describe the evolution of the stretching factor. Cottet et al. [8,9] showed that it is related to the gradient of a level set function transported by the physical velocity. We derive a generalization of this fact. For any extension of the physical velocity on the curve, the evolution of s_α can be expressed in a surprisingly simple way; see (2.2), (2.7). This fact allows us to incorporate the evolution of s_α along with the curve motion, without keeping track of the material coordinate α . In Sec. 3 we summarize the semi-Lagrangian contouring approach and outline the algorithm used in this work. The velocity solving the Stokes equations can be written as a singular integral (3.1) using the fundamental solution in a periodic box. Sec. 4 explains the Ewald splitting of this periodic fundamental solution, starting with splitting of the Green functions for the Laplacian and biharmonic operators. In Sec. 5 approximations are derived for

the local part of the Stokes velocity, with force on the curve, resulting in a single layer potential on the curve, or with a body force which has a jump at the curve, resulting in a convolution on the box.

In Sec. 6 we describe a test problem with an exact periodic solution of the elastic interface problem, (1.1), (1.6), (1.7), (1.11). The membrane is an ellipse which changes eccentricity in time. There is a body force which is discontinuous at the interface. In Sec. 7 our numerical results are presented...

In the immersed boundary method of Peskin [19], the fluid velocity is calculated on a grid; the force on the curve is spread to the grid points by replacing it with a sum of smoothed delta functions with a carefully designed shape. Although the method is generally first order, a second order version has been designed for the case where the interface is replaced by a layer of positive thickness [11]. Other papers concerned with the accuracy of the method include [18,20,31]. In [7] an alternate version was designed in which the smoothed delta functions are projected analytically onto the space of divergence-free vector fields, rather than discretizing first and projecting numerically, thereby removing an important source of error. In the method of [8,9] the location of the curve is found from a level set function advected with the fluid; the smoothed delta function is composed with the level set function. By contrast, in the methods of [15–17], the interface is sharp. The velocity is again computed on a regular grid, using finite differences, but the force at the interface is incorporated through the immersed interface method; that is, jump terms are added to the difference operators when the stencil crosses the boundary. A level set function was used for the curve motion in [17]. In the present work the interface is also sharp, but the interfacial curve is moved by the semi-Lagrangian contouring method and the velocity is computed from the integral representation. Recent work for boundary value problems [4,5] has aspects of several of these methods.

Boundary integral methods have been used extensively for Stokes flow in free space, in two or three dimensions, with different viscosities, to model particles, drops, or bubbles; see e.g. [21,22]. Most often the force is normal and proportional to curvature, as in the second term in (1.8). The integral formulation is natural, since the free space kernels are known explicitly, and since, with Stokes flow, the velocity is needed only on the moving boundary. However, if the velocity field is calculated at points on a regular grid in the fluid region, the integrals are nearly singular for points near the curve. The present method handles the more general task of computing the velocity at arbitrary points in periodic geometry. This capability will be needed if this approach is extended to Navier-Stokes flow.

In [13] the boundary integral method was used for moving boundaries in Stokes flow with equal arclength parametrization of the interface. With normal force,

it was found that the inherent stability requirement for explicit treatment of the boundary motion was $k \leq Ch$, where k is the time step and h is the spacing on the boundary. We expect that similar considerations apply with the general force (1.7), (1.8). However, stiffness may be a more serious problem with Navier-Stokes flow and with more general elastic response, e.g. as in [30].

The Ewald splitting of the Stokes velocity kernel is akin to regularization of the kernel of a singular or nearly singular integral with a local correction [2,3,6]. In fact, for the free space Laplacian, Gaussian regularization as in [2,3] gives the same splitting as the Ewald method [29]. Approximations for the local parts of nearly singular integrals have been derived in [2,3,10,29]. A general approach to Ewald splitting and local corrections for systems of elliptic equations has been developed in [23]. Cortez [6] used regularization of the Stokes fundamental solution in a variety of Stokes problems, with corrections from [2] added for forces on curves.

2 The stretching factor

?? this section is "finished"!

We describe the evolution of the stretching factor which occurs in the expression for the elastic boundary force. We suppose the moving curve $\Gamma(t)$ is parametrized by a material coordinate α , corresponding to arclength in the unstretched position. If $s = s(\alpha, t)$ is the arclength along the curve at the current time, the stretching factor is $s_\alpha(\alpha, t) = |X_\alpha(\alpha, t)|$, as in (1.10).

We suppose that a neighborhood of the curve is moved by a velocity field $V(x, t)$ which agrees with the physical velocity on $\Gamma(t)$ but may be different off the curve. Although the exact evolution of s_α depends only on the velocity on the curve, we will relate it to the extended velocity V and the signed distance function φ , introduced at time t_0 near $\Gamma(t_0)$. Thus each point x_0 nearby has the form $x_0 = X(\alpha, t_0) + \varphi(x_0, t_0)n(\alpha, t_0)$ for some α , where $n(\alpha, t_0)$ is the unit normal vector at $X(\alpha, t_0)$. Assuming $\Gamma(t_0)$ is C^2 , the inverse mapping $(\alpha, \varphi) \mapsto x_0$ is differentiable near $\Gamma(t_0)$. (These facts follow from the Tubular Neighborhood Theorem, with a similar statement for a surface in R^3 .) The determinant $\det(X_\alpha, X_\varphi)$ of the mapping $(\alpha, \varphi) \mapsto x_0$ at a point on the curve is $\pm|X_\alpha||n| = \pm|X_\alpha| = \pm s_\alpha$, since $X_\alpha \perp n$. The sign depends on the conventions for α, φ , and n .

Now suppose the curve and a neighborhood evolve in time according to the velocity $V(x, t)$, that is, $dx/dt = V(x, t)$ with $x(t_0; x_0) = x_0$. Let $J = J(x_0, t)$ be the Jacobian determinant of $\partial x/\partial x_0$. We can think of α, φ as coordinates for a neighborhood of $\Gamma(t)$ via the composition $(\alpha, \varphi) \mapsto x_0 \mapsto x$. The determinant

of this composition for $\phi = 0$ is $\pm J s_\alpha^0$, where s_α^0 is evaluated at x_0 at time t_0 . Using this fact we can express the derivative of the inverse function $x = (x_1, x_2) \mapsto (\alpha, \varphi)$ as the inverse matrix of the derivative of $(\alpha, \varphi) \rightarrow x$,

$$\begin{pmatrix} \partial_1 \alpha & \partial_2 \alpha \\ \partial_1 \varphi & \partial_2 \varphi \end{pmatrix} = \frac{1}{\pm J s_\alpha^0} \begin{pmatrix} x_{2,\varphi} & -x_{1,\varphi} \\ -x_{2,\alpha} & x_{1,\alpha} \end{pmatrix}. \quad (2.1)$$

From the second row of this formula we see that $|\nabla \varphi| = |X_\alpha|/(J s_\alpha^0)$. Solving for $s_\alpha = |X_\alpha|$, we have $s_\alpha = |\nabla \varphi| J s_\alpha^0$. More explicitly, for a material point on the curve, for which the marker α is preserved by the flow,

$$s_\alpha(\alpha, t) = |\nabla \varphi(x, t)| J(x_0, t) s_\alpha(\alpha, t_0), \quad x_0 = X(\alpha, t_0), \quad x = X(\alpha, t). \quad (2.2)$$

Thus the stretching s_α at later time t is determined by its initial value, the mapping induced by V , and $\nabla \varphi$, which in turn is determined by the mapping. Further simplification depends on the choice of V . If V is the physical velocity, with $\nabla \cdot V \equiv 0$, then $J \equiv 1$, and (2.2) reduces to $s_\alpha(\alpha, t) = |\nabla \varphi(x, t)| s_\alpha(\alpha, t_0)$ as shown by Cottet et al. [9], Cor. 2.1 and [8], Lemma 3.1.

For a surface in \mathbf{R}^3 , (2.2) has a direct analogue with entirely similar derivation. If the material coordinates are $\alpha = (\alpha_1, \alpha_2)$, the stretching factor is $s_\alpha = |(\partial X/\partial \alpha_1) \times (\partial X/\partial \alpha_2)|$. The 3D analogue of (2.1) has as its third row the equation $\nabla \varphi = (X_{\alpha_1} \times X_{\alpha_2})/(J s_\alpha^0)$, leading again to the formula (2.2).

2.1 Stretching with normal velocity extension

We now assume that the velocity field $V(x, t)$ is extended from the curve so that its normal derivative is zero on the curve at each time t ,

$$(n \cdot \nabla) V(x, t) = 0, \quad x \in \Gamma(t). \quad (2.3)$$

Then, since $|\nabla \varphi| \equiv 1$ at time t_0 on the curve $\Gamma(t_0)$, the same is true at later time as well,

$$|\nabla \varphi(x, t)| = 1, \quad x \in \Gamma(t). \quad (2.4)$$

This is essentially the observation of Lemma A.1 in [32]; it is readily verified by differentiating $|\nabla \phi|^2$ in time. In this case the formula (2.2) for the stretching reduces to

$$s_\alpha(\alpha, t) = J(x_0, t) s_\alpha(\alpha, t_0). \quad (2.5)$$

Moreover, it is a standard fact that

$$\frac{d}{dt} J(x_0, t) = \nabla \cdot V(x, t) J(x_0, t). \quad (2.6)$$

Thus, with assumption (2.3) we have the following simple differential form of the stretching law

$$\frac{d}{dt}s_\alpha(\alpha, t) = \nabla \cdot V(x, t) s_\alpha(\alpha, t), \quad x = X(\alpha, t). \quad (2.7)$$

We use this equation to evolve s_α in our scheme.

3 The numerical method

?? J, see if you like the first part, esp. as related ?? to the rest of the paper ?? You will want to revise the description of your method ?? Check whether the 12 steps need revision ?? stretching factor is called sal, currently set to q

At each time we need to find the location of the curve Γ and the stretching factor s_α . The curve moves with the velocity field v , determined from (1.1). The interfacial force in (1.7)–(1.9) is determined by s_α . Our procedure for moving the curve uses an extension of the velocity of the curve along normal lines, rather than the physical velocity. In this case condition (2.3) holds, and we can use (2.7) to update s_α .

The velocity in Stokes flow has an integral representation derived from potential theory, in terms of the (periodic) fundamental solution S_{ij} of the Stokes equations (e.g., see [22]). The velocity $v = (v_1, v_2)$ defined in the periodic domain Q solving (1.1) is

$$v_i(y) = \int_\Gamma S_{ij}(y - x(s))f_j(s) ds + \int \int_Q S_{ij}(y - x)F_{bj}(x) dx_1 dx_2 \quad (3.1)$$

with sum over $j = 1, 2$. This representation is derived in Sec. 4, and the method for computing the velocity is described in Secs. 4 and 5. To find the motion of Γ we need only compute the velocity on Γ , but the full velocity field can be found as needed.

The motion of the interface is computed using a method developed in [24–28] which combines the following modules:

Distancing. Given the curve Γ , a distance tree is built near Γ , that is, a quadtree mesh consisting of square cells on several levels, with pointers to nearby elements of Γ . In building the tree, cells are split if a larger concentric cell intersects Γ . The signed distance function φ is known on the vertices of the tree, and interpolated to other points. (See Sec. 1.3 of [25], and for more detail in an earlier version, Secs. 3 and 4 of [26].)

Velocity extension. Given the velocity v on the curve Γ , values are extended

to the vertices of the tree by finding the nearest point on Γ and assigning its velocity. The extended velocity V at an arbitrary point is found by interpolation. This is a numerical version of the Whitney extension procedure. (See [25], Sec. 2.)

Advection. Given the signed distance function φ on the curve Γ and the extended velocity V , solve approximately the advection equation

$$\varphi_t + V \cdot \nabla \varphi = 0$$

from time t to $t + k$ by the semi-Lagrangian, or CIR, method. That is, given \tilde{x} , define

$$\psi(\tilde{x}) = \varphi(\tilde{x} - kV(\tilde{x})).$$

The predicted curve $\tilde{\Gamma}$ at time $t + k$ will be the zero set of ψ . (For the second-order version in predictor-corrector form, see [25], Sec. 1.2, or steps (4),(9),(10) below.)

Contouring. Given the advected level set function ψ , find its zero set $\tilde{\Gamma}$: Introduce a new tree, splitting each cell whose length exceeds the minimum value of ψ on the cell. Triangulate the cells and find the zero set of the piecewise linear interpolant of ψ . Move each vertex to reduce $|\psi|$ at the vertex below a specified tolerance. Split segments as needed to reduce $|\psi|$ between vertices. (See [24], Sec. 2.)

We can now summarize our procedure. We denote the function s_α on the curve by q . We outline one time step from time t to $t + k$:

- (0) At time t we know the curve Γ , the associated signed distance function φ , the tree T , and the stretching factor q on Γ .
- (1) Introduce a fine local mesh near Γ . Compute the normal n (equivalently tangent τ), and curvature κ . Compute the force f on the curve Γ , using (1.8), (1.11).
- (2) From f on Γ , and possibly a body force $F_b(t)$, find the velocity v on Γ from (3.1).
- (3) Extend v to V on the tree T for the curve Γ .
- (4) Find $\tilde{\Gamma}$ as the set of \tilde{x} with $\varphi(x) = 0$, where $x = \tilde{x} - kV(\tilde{x})$.
- (5) Build new tree \tilde{T} and compute $\tilde{\varphi}$, the signed distance function to $\tilde{\Gamma}$, on \tilde{T} .
- (6) Find $\nabla \cdot V(x)$ for $x \in \Gamma$ via a local mesh on Γ . Update q to $\tilde{q}(\tilde{x}) = (1 + k\nabla \cdot V(x))q(x)$ for \tilde{x} on $\tilde{\Gamma}$. (This completes the predictor half-cycle.)

(7) Introduce a local mesh near $\tilde{\Gamma}$. Compute the new normal, tangent, curvature, and the force \tilde{f} on the curve $\tilde{\Gamma}$, determined by \tilde{q} .

(8) From \tilde{f} on $\tilde{\Gamma}$, and possibly a body force $F_b(t+k)$, find the velocity \tilde{v} on $\tilde{\Gamma}$ using (3.1).

(9) Extend \tilde{v} to \tilde{V} on the tree \tilde{T} for the curve $\tilde{\Gamma}$. Set $\bar{V}(\bar{x}) = \frac{1}{2}\tilde{V}(\bar{x}) + \frac{1}{2}V(\bar{x} - kV(\bar{x}))$ on \tilde{T} .

(10) Find $\bar{\Gamma}$ as the set of \bar{x} with $\varphi(x) = 0$, where $x = \bar{x} - k\bar{V}(\bar{x})$.

(11) Build new tree \bar{T} and compute $\bar{\varphi}$, the signed distance function to $\bar{\Gamma}$, on \bar{T} .

(12) For $x \in \Gamma$ find $\nabla \cdot V(x)$ via a local mesh on Γ . ?? John is this needed?? For $\bar{x} \in \bar{\Gamma}$ find $\nabla \cdot \tilde{V}(\bar{x})$ via a local mesh on $\bar{\Gamma}$. For $\bar{x} \in \bar{\Gamma}$, update q , with $x = \bar{x} - k\bar{V}(\bar{x})$ as in (10),

$$\bar{q}(\bar{x}) = q(x) + \frac{1}{2}k\nabla \cdot V(x)q(x) + \frac{1}{2}k\nabla \cdot \tilde{V}(\bar{x})\bar{q}(\bar{x})$$

with the last term locally implicit, or equivalently

$$\bar{q}(\bar{x}) = \frac{1 + \frac{1}{2}k\nabla \cdot V(x)}{1 - \frac{1}{2}k\nabla \cdot \tilde{V}(\bar{x})}q(x)$$

(This ends the complete cycle.)

4 Ewald summation for Stokes flow

?? section 4 is "finished"! ?? Ewald parameter (formerly tau) is called ew, currently sigma

4.1 The steady Stokes equations

The steady Stokes equations on a d -dimensional periodic box $Q = [-\pi, \pi]^d \subset R^d$ for the velocity $v : Q \rightarrow R^d$ and pressure $p : Q \rightarrow R$ are

$$-\nu\Delta v + \nabla p = F, \quad \nabla \cdot v = 0, \quad (4.1)$$

where F is a force with mean zero (for consistency). Applying the divergence operator yields $\Delta p = \nabla \cdot F = \partial_j F_j$, and substituting back in gives a biharmonic equation

$$\nu\Delta^2 v_i = \partial_i \partial_j F_j - \Delta F_i \quad (4.2)$$

where $\partial_i = \partial/\partial x_i$ and repeated indices imply summation. Let

$$\Delta G = \delta - 1/|Q|, \quad \int_0 G dx = 0, \quad (4.3)$$

define the periodic mean-zero Green function for the Laplace equation and

$$\Delta B = G, \quad \int_Q B dx = 0, \quad (4.4)$$

define the periodic mean-zero Green function for the biharmonic equation, with $|Q| = (2\pi)^d$. Then

$$\nu v_i = \partial_i \partial_j B \star F_j - \Delta B \star F_i. \quad (4.5)$$

We now seek convenient formulas for G , B and $\partial_i \partial_j B$.

4.2 Ewald summation for the Laplacian

The obvious Fourier series

$$G(x) = -(2\pi)^{-d} \sum_{k \neq 0} \frac{1}{|k|^2} e^{ik \cdot x} \quad (4.6)$$

for G does not converge quickly enough to be useful in computation. Ewald summation expresses G as the sum of two rapidly converging series, one smooth and one singular but localized. The technique can be derived in a variety of ways which suggest various extensions. The following derivation appears to be new. Let K_t be the fundamental solution of the periodic heat equation given in two different forms as

$$K_t(x) = (2\pi)^{-d} \sum_k e^{-t|k|^2} e^{ik \cdot x} = (4\pi t)^{-d/2} \sum_{m \in Z^d} e^{-r_m^2/4t}, \quad (4.7)$$

where $r_m = |x - 2\pi m|$. As $t \rightarrow 0$, $K_t(x) \rightarrow K_0(x) = \delta(x)$, a periodic delta function as $t \rightarrow 0$. Note that K_t has mean $1/|Q|$ for all $t \geq 0$. Fix a smoothing parameter $\sigma > 0$ and write

$$\begin{aligned} G &= G \star (\delta - 1/|Q|) = G \star (K_\sigma - 1/|Q|) + G \star (\delta - K_\sigma) \\ G \star (\delta - K_\sigma) &= G \star (K_0 - K_\sigma) = -G \star \int_0^\sigma \partial_t K_t dt \\ &= -G \star \int_0^\sigma \Delta K_t dt = -\int_0^\sigma K_t dt + \sigma/|Q|. \end{aligned}$$

Finally we write G as the sum $G = G^F + G^L$ of Fourier and local parts, with G^F defined as

$$G^F = G \star (K_\sigma - 1/|Q|) + \sigma/|Q| \quad (4.8)$$

so that

$$G^F(x) = (2\pi)^{-d} \left(\sigma - \sum_{k \neq 0} \frac{e^{-\sigma|k|^2}}{|k|^2} e^{ik \cdot x} \right). \quad (4.9)$$

The $k = 0$ term in the Fourier series for G^F is nonzero. This does not matter when convolving with a function F which has mean zero, but will make a difference when evaluating pointwise values of the full Green function.

By integration, we find the complementary local part,

$$G^L(x) = - \int_0^\sigma K_t(x) dt = - \sum_m \int_0^\sigma (4\pi t)^{-d/2} e^{-r_m^2/4t} dt \quad (4.10)$$

$$= -\frac{1}{4} \pi^{-d/2} \sum_m r_m^{2-d} \Gamma\left(d/2 - 1, \frac{r_m^2}{4\sigma}\right). \quad (4.11)$$

Here $\Gamma(a, z) = \int_z^\infty e^{-s} s^{a-1} ds$ is the usual incomplete gamma function, which is appropriately singular as $z \rightarrow 0$ but decays exponentially as $z \rightarrow \infty$. Thus we can usually omit the images $2\pi m$ whenever x is well inside the box Q .

4.3 Biharmonic Ewald summation by squaring

The straightforward approach to Ewald summation for the biharmonic equation requires the inverse Fourier transform of $e^{-t|k|^4}$, which is difficult to evaluate. Thus we consider two different approaches, both based on the Ewald splitting of the Green function G for Laplacian, which we call squaring and subtraction. The second is used in the present work. In the squaring approach, we observe that

$$\begin{aligned} B &= G \star G = (G^F + G^L) \star (G^F + G^L) \\ &= G^F \star (G^F + 2G^L) + G^L \star G^L \equiv B^F + B^L \end{aligned}$$

where (since convolution multiplies Fourier coefficients)

$$B^F(x) = (2\pi)^{-d} \left(-\sigma^2 + \sum_{k \neq 0} \frac{e^{-\sigma|k|^2} (2 - e^{-\sigma|k|^2})}{|k|^4} e^{ik \cdot x} \right) \quad (4.12)$$

and

$$B^L(x) = \int_0^\sigma \int_0^\sigma (K_t \star K_s)(x) ds dt = \int_0^\sigma \int_0^\sigma K_{t+s}(x) ds dt \quad (4.13)$$

since the heat kernel defines a semigroup. Consider $G^L(x; \sigma)$ as a function of the smoothing parameter σ , (as well as x) and let $H(x; t) = \int_0^t G^L(x; \sigma) d\sigma$ be

an antiderivative; then

$$B^L(x) = \int_0^\sigma \partial_t H(x; t + \sigma) - \partial_t H(x; t) dt = H(2\sigma) - 2H(\sigma) \quad (4.14)$$

where a tedious calculation gives

$$H(t) = \frac{1}{16\pi^{d/2}} \sum_m r_m^{4-d} \left(\frac{4t}{r_m^2} \Gamma\left(d/2 - 1, \frac{r_m^2}{4t}\right) + \Gamma\left(d/2 - 2, \frac{r_m^2}{4t}\right) \right) \quad (4.15)$$

4.4 Biharmonic Ewald summation by subtraction

We can use a more direct approach in which the local part of the biharmonic Ewald sum is defined by modifying the free-space Green function in a way that preserves the local singularity. We take the two-dimensional case $d = 2$ for simplicity. The free-space Green function for the Laplace equation is

$$G_\infty(x) = \frac{1}{2\pi} \log |x|, \quad (4.16)$$

and the corresponding free-space Green function for the biharmonic is

$$B_\infty(x) = \frac{1}{8\pi} |x|^2 (\log |x| - 1). \quad (4.17)$$

The derivation of harmonic Ewald summation and the singularity

$$\Gamma(0, z) = \int_z^\infty e^{-s} \frac{ds}{s} \sim -\log z \quad \text{as } z \rightarrow 0$$

suggests that we *define*

$$B^L(x) = -\frac{1}{16\pi} \sum_{m \in \mathbb{Z}^2} r_m^2 \Gamma\left(0, \frac{r_m^2}{4\sigma}\right) \quad (4.18)$$

to provide a periodic rapidly-decaying function which matches the local singularity of B . We then use the Poisson summation formula to evaluate the smooth part $B^F = B - B^L$ as a Fourier series. Note that neither B^F nor B^L have mean zero, but their sum B does. Reversing the computation of $G^L(x)$ shows that

$$\begin{aligned} B^L(x) &= -\frac{1}{4} \int_0^\sigma \sum_m r_m^2 (4\pi t)^{-1} e^{-r_m^2/4t} dt \\ &= -\frac{1}{4\pi} \int_0^\sigma t \frac{d}{dt} \sum_m e^{-r_m^2/4t} dt = -(2\pi)^{-2} \sum_k \int_0^\sigma t \frac{d}{dt} (te^{-t|k|^2}) dt e^{ik \cdot x} \end{aligned}$$

where we have integrated by parts and used the equality (4.7), a case of the Poisson summation formula. Then, since $B^F = B - B^L$ and

$$B(x) = (2\pi)^{-2} \sum_{k \neq 0} \frac{1}{|k|^4} e^{ik \cdot x}, \quad (4.19)$$

we obtain the rapidly converging Fourier series for B^F ,

$$B^F(x) = (2\pi)^{-2} \left(\frac{\sigma^2}{2} + \sum_{k \neq 0} \frac{1}{|k|^4} (1 + \sigma|k|^2 + \sigma^2|k|^4) e^{-\sigma|k|^2} e^{ik \cdot x} \right). \quad (4.20)$$

Its second partial derivatives are given by

$$\partial_i \partial_j B^F(x) = -(2\pi)^{-2} \sum_{k \neq 0} \frac{k_i k_j}{|k|^4} (1 + \sigma|k|^2 + \sigma^2|k|^4) e^{-\sigma|k|^2} e^{ik \cdot x}. \quad (4.21)$$

4.5 Application to the Stokes velocity

The decomposition $B = B^F + B^L$ above leads to a corresponding decomposition of the operator producing the Stokes velocity into a smooth part and a local part. We write (4.5) in the form

$$\nu v_i = \Sigma_j S_{ij} \star F_j \quad (4.22)$$

with

$$S_{ij} = \partial_i \partial_j B - \delta_{ij} \Delta B. \quad (4.23)$$

It is natural to write S_{ij} as the sum

$$S_{ij} = S_{ij}^F + S_{ij}^L \quad (4.24)$$

with

$$S_{ij}^F = \partial_i \partial_j B^F - \delta_{ij} \Delta B^F, \quad (4.25)$$

$$S_{ij}^L = \partial_i \partial_j B^L - \delta_{ij} \Delta B^L. \quad (4.26)$$

The smooth part S^F has the Fourier representation

$$S_{ij}^F(x) = (2\pi)^{-2} \sum_{k \neq 0} s_{ij}(k) e^{ik \cdot x}, \quad (4.27)$$

$$s_{ij}(k) = \frac{\delta_{ij}|k|^2 - k_i k_j}{|k|^4} (1 + \sigma|k|^2 + \sigma^2|k|^4) e^{-\sigma|k|^2}. \quad (4.28)$$

The local part will be written explicitly in the next section.

5 Computation of the Stokes velocity

?? Section 5 is "finished"! ?? tangent is tnt, currently set to tau

In the last section the velocity v , determined by the Stokes equations (4.1), with given force F , was written as the convolution

$$\nu v_i = \sum_j S_{ij} \star F_j. \quad (5.1)$$

The velocity kernel S , given by (4.23), was decomposed into a smooth part and a local part, $S = S^F + S^L$. The two parts will be treated separately. For convenience we write the velocity as $v = v^F + v^L$.

5.1 The Fourier part

The velocity term v^F contributed by the smooth part of the kernel is computed as a Fourier series. The method is similar to that of [29]. Writing F in a Fourier series,

$$F(x) = \sum_k \hat{F}(k) e^{ikx}, \quad \hat{F}(k) = (2\pi)^{-2} \int_Q F(x) e^{-ikx} dx \quad (5.2)$$

and using the Fourier representation (4.27,4.28) of S^F , we have

$$\nu v_i^F(x) = \sum_j \sum_k s_{ij}(k) \hat{F}_j(k) e^{ikx}. \quad (5.3)$$

Because of the exponential decay of $s_{ij}(k)$ in (4.28) we can truncate the series. We choose parameter p and sum over $k = (k_1, k_2)$ with $|k_1|, |k_2| \leq p$. The error E_F due to this truncation is at most

$$|E_F| \leq \sqrt{2\pi} \frac{e^{-p^2\sigma}}{p^3\sigma^{3/2}}. \quad (5.4)$$

(See [29], p. 253.) The estimate depends only on $p^2\sigma$. For example, $p^2\sigma = 20$ gives an error less than 10^{-10} .

?? John, see if what's below should be revised?? If the force F is on the curve, in the form $F = f\delta_\Gamma$, the Fourier coefficient of F is an integral over the curve,

$$\hat{F}(k) = (2\pi)^{-2} \int_\Gamma f(x) e^{-ikx} dx(s). \quad (5.5)$$

We compute these coefficients by a quadrature rule over the line segments of which Γ is constructed. (Compare [29], p. 255.) If F is a body force, we use a trapezoidal rule for the integral (5.5). If F has a jump discontinuity at Γ , we

approximate Γ by a line segment in each grid square it cuts and choose some value of F on the correct side for each part of the square.

5.2 The local part

We derive approximations to the contribution v^L valid for small σ . This is possible because the kernel S^L has Gaussian decay away from the singularity. It is convenient to replace the Ewald parameter σ with a new parameter δ , defined by

$$\delta^2 = 4\sigma. \quad (5.6)$$

It is the radius of smoothing in G^F and B^F and the length scale for the decay in S^L . We obtain an expansion in powers of δ . Similar expansions have been used in [10],[29],[2], [3]. The analytical technique here is close to that in [2].

We ignore the periodic reflections in the formulas (4.11,4.18) for G^L , B^L , presuming that the sources are well inside the periodic boundary. Thus, with $r = |x|$,

$$G^L(r) \approx -\frac{1}{4\pi}\Gamma(0, r^2/\delta^2), \quad B^L(r) \approx -\frac{r^2}{16\pi}\Gamma(0, r^2/\delta^2). \quad (5.7)$$

Corresponding to B^L , the local part of the Stokes velocity is $v_i^L = \Sigma_j S_{ij}^L \star F_j$ with

$$S_{ij}^L = \partial_i \partial_j B^L - \delta_{ij} \Delta B^L. \quad (5.8)$$

To obtain detailed expressions we start with derivatives of G^L , B^L :

$$\partial_r G^L = \frac{1}{2\pi r} e^{-r^2/\delta^2} \quad (5.9)$$

$$\partial_j B^L = \frac{1}{4} \left(2x_j G^L + \frac{x_j}{2\pi} e^{-r^2/\delta^2} \right) \quad (5.10)$$

and with $\rho = r/\delta$,

$$\partial_i \partial_j B^L = \delta_{ij} \left(\frac{1}{2} G^L + \frac{e^{-\rho^2}}{8\pi} \right) + \frac{x_i x_j}{4\pi r^2} (1 - \rho^2) e^{-\rho^2} \quad (5.11)$$

and in particular

$$\Delta B^L = \sum_j \partial_j^2 B^L = G^L + \frac{1}{2\pi} \left(1 - \frac{\rho^2}{2} \right) e^{-\rho^2}. \quad (5.12)$$

Now substituting (5.11,5.12) in (4.26) we can write S^L explicitly as

$$S_{ij}^L = -\frac{\delta_{ij}}{2} G^L + \delta_{ij} e^{-\rho^2} \left(-\frac{3}{8\pi} + \frac{\rho^2}{4\pi} \right) + \frac{x_i x_j}{4\pi r^2} (1 - \rho^2) e^{-\rho^2} \quad (5.13)$$

To proceed further we consider separately the two cases of the force.

5.3 The local integral over a curve

We now analyze the local part of velocity v^L when $F = f\delta_\Gamma$, representing a force f on a curve Γ . At an arbitrary point y

$$\nu v_i^L(y) = \int_\Gamma \sum_j S_{ij}^L(y - x(s)) f_j(s) ds \quad (5.14)$$

where s is the arclength parameter on the curve. We will derive an approximation valid to $O(\delta^3)$. Since S^L is localized we are only concerned with y near the curve Γ and the part of the integral with $x(s)$ near y . For such y we can write $y = x(s_0) + bn(s_0)$ where $x(s_0)$ is a point on Γ and $n(s_0)$ is the unit normal at that point. For simplicity we assume $s_0 = 0$. We write $\tau = x'(0)$ for the unit tangent, and $n = n(0)$ for the normal, denoting the s -derivative with $'$. We have $x''(0) = -\kappa n$, where κ is the curvature at $x(0)$.

We use Taylor expansions in s and b to identify the largest terms in (5.14). We begin with

$$x(s) - y = \tau s - \left(\frac{1}{2}\kappa s^2 + b\right)n + O(s^3). \quad (5.15)$$

Let $r^2 = |x(s) - y|^2$ and $R^2 = s^2 + b^2$. Then

$$r^2 = s^2 + b^2 + \kappa b s^2 + O(R^4) \quad (5.16)$$

We now introduce a new variable $\xi = \xi(s, b)$ defined by $r^2 = \xi^2 + b^2$ in order to simplify the dependence of the integrand on r . Solving for ξ in (5.16) we have $\xi^2 = (1 + \kappa b)s^2 + O(R^4)$ or

$$\xi = \left(1 + \frac{1}{2}\kappa b\right)s + O(R^3). \quad (5.17)$$

We can now solve for $s = s(\xi, b)$, obtaining

$$s = \left(1 - \frac{1}{2}\kappa b\right)\xi + O(r^3) \quad (5.18)$$

and

$$\frac{ds}{d\xi} = 1 - \frac{1}{2}\kappa b + O(r^2). \quad (5.19)$$

Now substituting for s in terms of ξ in (5.15) we get

$$x(s) - y = \left(1 - \frac{1}{2}\kappa b\right)\xi\tau - \left(\frac{1}{2}\kappa\xi^2 + b\right)n + O(r^3) \quad (5.20)$$

and similarly for f

$$f = f(0) + f'(0)s + O(s^2) = f(0) + f'(0)\xi + O(r^2). \quad (5.21)$$

In evaluating various parts of the integral (5.14) we use the substitution $\xi = \delta\zeta$ and $b = \delta\beta$, noting that $\rho = r/\delta = \sqrt{\zeta^2 + \beta^2}$. Four integrals related to the Gaussian will be needed. If

$$I_p = \int_{-\infty}^{\infty} \frac{e^{-(\zeta^2 + \beta^2)}}{\zeta^2 + \beta^2} \zeta^p d\zeta, \quad J_p = \int_{-\infty}^{\infty} e^{-(\zeta^2 + \beta^2)} \zeta^p d\zeta, \quad (5.22)$$

then

$$I_0 = (\pi/|\beta|) \operatorname{erfc}|\beta|, \quad I_2 = \sqrt{\pi} e^{-\beta^2} - \pi|\beta| \operatorname{erfc}|\beta|, \quad (5.23)$$

$$J_0 = \sqrt{\pi} e^{-\beta^2}, \quad J_2 = (\sqrt{\pi}/2) e^{-\beta^2}. \quad (5.24)$$

We begin with the integral of $G^L f_i$, corresponding to the part of (5.14) coming from the first term of (5.13):

$$\begin{aligned} \int G^L(r/\delta) f_i \frac{ds}{d\xi} d\xi &= \int G^L(r/\delta) \left[(f_{0i} + f'_{0i}\xi) (1 - \frac{1}{2}\kappa b) + O(r^2) \right] d\xi \\ &= (1 - \frac{1}{2}\kappa b) f_{0i} \int G^L(r/\delta) d\xi + \text{odd term} + \text{remainder} \end{aligned} \quad (5.25)$$

We evaluate the last integral as follows:

$$\begin{aligned} \int G^L(r/\delta) d\xi &= \delta \int G^L(\rho) d\zeta = -\delta \int \frac{\partial G^L}{\partial \zeta} \zeta d\zeta \\ &= -\delta \int \frac{\partial G^L}{\partial \rho} \frac{\zeta}{\rho} \cdot \zeta d\zeta = -\delta \int \frac{1}{2\pi\rho} e^{-\rho^2} \frac{\zeta^2}{\rho} d\zeta = -\frac{\delta}{2\pi} I_2. \end{aligned}$$

The term in (5.25) with $f'_{0i}\xi$ is odd in ξ and integrates to 0. The $O(r^2)$ remainder in (5.25) is a sum of terms, each a monomial of degree 2 in ξ, b times a bounded function, and the integral is $O(\delta \cdot \delta^2) = O(\delta^3)$. Thus

$$A_{1i} \equiv \int G^L(r/\delta) f_i ds = -\frac{\delta}{2\pi} (1 - \frac{1}{2}\kappa b) I_2 f_{0i} + O(\delta^3) \quad (5.26)$$

Looking at the next terms in (5.13) we see in a similar but simpler way that

$$A_{2i} \equiv \int e^{-\rho^2} f_i d\xi = \delta (1 - \frac{1}{2}\kappa b) J_0 f_{0i} + O(\delta^3), \quad (5.27)$$

$$A_{3i} \equiv \int e^{-\rho^2} \rho^2 f_i d\xi = \delta (1 - \frac{1}{2}\kappa b) (J_2 + \beta^2 J_0) f_{0i} + O(\delta^3). \quad (5.28)$$

To handle the remaining part of S^L , we note that

$$\sum_j (x_j - y_j) f_j = (1 - \frac{1}{2}\kappa b) (f_\tau \xi + f'_\tau \xi^2) - (\frac{1}{2}\kappa \xi^2 + b) (f_n + f'_n \xi) + O(r^3)$$

where $f_\tau = \sum_j f_{0j} \tau_j$, $f_n = \sum_j f_{0j} n_j$ and similarly f'_τ, f'_n are tangential and

normal components of f'_0 . Then

$$\begin{aligned} \sum_j (x_i - y_i)(x_j - y_j) f_j \frac{ds}{d\xi} &= (1 - \frac{3}{2}\kappa b)\xi^2 f_\tau \tau_i + (b^2 - \frac{1}{2}\kappa b^3 + b\kappa\xi^2) f_n n_i \\ &\quad - b\xi^2 (f'_n \tau_i + f'_\tau n_i) + \text{odd terms} + O(r^4) \end{aligned}$$

and proceeding as with the earlier terms we find, with $M_p = I_p - J_p$,

$$\begin{aligned} A_{4i} &\equiv \int \sum_j \frac{(x_i - y_i)(x_j - y_j)}{r^2} (1 - \rho^2) e^{-\rho^2} f_j d\xi \\ &= \delta(1 - \frac{3}{2}\kappa b) M_2 f_\tau \tau_i + \delta\beta^2(1 - \frac{1}{2}\kappa b) M_0 f_n n_i + \delta^2\beta\kappa M_2 f_n n_i \\ &\quad - \delta^2\beta M_2 (f'_n \tau_i + f'_\tau n_i) + O(\delta^3). \end{aligned} \quad (5.29)$$

We can now substitute (5.26)–(5.29) into (5.13), (5.14) to get an expression for the local part of the velocity,

$$\nu v_i^L = -\frac{1}{2}A_{1i} - \frac{3}{8\pi}A_{2i} + \frac{1}{4\pi}A_{3i} + \frac{1}{4\pi}A_{4i} + O(\delta^3). \quad (5.30)$$

It is convenient to combine the first three terms and rewrite this as

$$4\pi\nu v_i^L = \delta(1 - \frac{1}{2}\kappa b) (I_2 - (1 - \beta^2)J_0) f_{0i} + A_{4i} + O(\delta^3). \quad (5.31)$$

In the special case when $b = 0$, i.e. y is on the curve, this expression simplifies to

$$4\pi\nu v_i^L = \frac{1}{2}\delta\sqrt{\pi} f_\tau \tau_i + O(\delta^3) \quad (5.32)$$

5.4 The local integral of a body force

Next we approximate the local velocity resulting from a body force F which may be discontinuous across a curve Γ . We first suppose that F is nonzero only inside the domain D bounded by Γ . In place of (5.14) we have the integral

$$\nu v_i^L(y) = \int \int_D \sum_j S_{ij}^L(y - x) F_j(x) dx_1 dx_2. \quad (5.33)$$

If y is away from Γ , it can be seen that this local velocity is $O(\delta^4)$ because of the form (5.8) for S^L in second derivatives of B^L ; the fact that B^L in (5.7) is δ^2 times a function of $\rho = r/\delta$; and the rapid decay of B^L . For this reason we consider a point y near the curve. For simplicity we assume y is along a vertical normal line to the curve at distance b , and we set $y = (0, 0)$. Thus we suppose the curve has the form

$$x_2 = Y(x_1) = -b + \frac{1}{2}Y''_0 x_1^2 + O(x_1^3) \quad (5.34)$$

so that the curve passes through $(0, -b)$ with normal $(0, 1)$. The integrand is significant only for x near 0. Assuming b is small, we introduce new coordinates $\xi = (\xi_1, \xi_2)$ so that the exterior $x_2 > Y(x_1)$ corresponds to $\xi_2 > -b$ and the radial distance is preserved, that is,

$$\xi_1^2 + \xi_2^2 = x_1^2 + x_2^2 \equiv r^2. \quad (5.35)$$

Given x we first define ξ_2 as

$$\xi_2 = x_2 - Y(x_1) - b = x_2 - \frac{1}{2}Y_0''x_1^2 + O(x_1^3) \quad (5.36)$$

so that (5.35) reduces to $\xi_1^2 = x_1^2 + 2\xi_2(Y + b) + (Y + b)^2$. Since $(Y + b)/x_1^2$ is smooth, this equation defines ξ_1 , with the convention that ξ_1 and x_1 have the same sign. We have $\xi_1^2 = x_1^2(Y_0''\xi_2 + O(x))$ or

$$\xi_1 = (1 + \frac{1}{2}Y_0''\xi_2)x_1 + O(x^2). \quad (5.37)$$

From the approximations (5.36,5.37) it follows that

$$x = \xi + O(r^2), \quad J \equiv \det\left(\frac{\partial x}{\partial \xi}\right) = 1 + O(r). \quad (5.38)$$

We now convert the integral (5.33) to the new variables,

$$\nu v_i^L = \int_{-\infty}^{-b} \int_{-\infty}^{\infty} \sum_j S_{ij}^L(x) F_j(x) J d\xi_1 d\xi_2 \quad (5.39)$$

and note that the dependence on r/δ is unaffected by the conversion. We will evaluate to $O(\delta^3)$. We will make crude approximations, and it will become evident that further terms are of the order neglected. Thus we replace $F_j(x)$ with $F_{0j} = F_j(0, 0)$ and J with 1. We ignore the distinction between x and ξ , obtaining

$$\nu v_i^L \approx \int_{-\infty}^{-b} \int_{-\infty}^{\infty} \sum_j S_{ij}^L(x) F_{0j} dx_1 dx_2. \quad (5.40)$$

For $i = 2$ we can use (5.8) to write the integrand as $\partial_{21}B^L F_{01} - \partial_{11}B^L F_{02}$; since this is an x_1 -derivative, the integral is zero. For $i = 1$, the integrand is $\partial_{12}B^L F_{02} - \partial_{22}B^L F_{01}$; the first term again integrates to zero, and for the same reason we can replace the second term by $-(\Delta B^L)F_{01}$. We now have

$$\nu v_1^L \approx -F_{01} \int_{-\infty}^{-b} \int_{-\infty}^{\infty} \Delta B^L dx_1 dx_2. \quad (5.41)$$

One term in ΔB^L is G^L . We rewrite the x_1 -integral of this term as

$$\int_{-\infty}^{\infty} G^L(x_1, x_2) dx_1 = - \int_{-\infty}^{\infty} x_1 \frac{dG^L}{dx_1} dx_1 = - \int_{-\infty}^{\infty} \frac{x_1^2}{2\pi r^2} e^{-r^2/\delta^2} dx_1$$

Substituting from (5.12) and combining terms we have

$$\nu v_1^L \approx \frac{F_{01}}{2\pi} \int_{-\infty}^{-b} \int_{-\infty}^{\infty} \left(\frac{-x_2^2}{x_1^2 + x_2^2} + \frac{1}{2}(x_1^2 + x_2^2) \right) e^{-r^2/\delta^2} dx_1 dx_2.$$

We now rescale the variables, $(x_1, x_2) \mapsto (\delta x_1, \delta x_2)$. and set $\beta = b/\delta$, so that

$$\nu v_1^L \approx \frac{\delta^2 F_{01}}{2\pi} \int_{-\infty}^{-\beta} \int_{-\infty}^{\infty} \left(\frac{-x_2^2}{x_1^2 + x_2^2} + \frac{1}{2}(x_1^2 + x_2^2) \right) e^{-r^2} dx_1 dx_2.$$

We note that the integrand is even in x_2 and the integral from 0 to ∞ is zero. Thus for $\beta > 0$, the integral from $-\infty$ to $-\beta$ is minus that from 0 to β , and for $\beta < 0$, the integral is equal to that from 0 to $|\beta|$. Evaluating the integral we find

$$\nu v_1^L \approx -\frac{\delta^2 F_{01}}{8\pi} \beta \left(\sqrt{\pi} e^{-\beta^2} - 2\pi |\beta| \operatorname{erfc}|\beta| \right). \quad (5.42)$$

The term just found was $O(\delta^2)$ because of the rescaling of the area form. If we considered further terms we would have additional factors of ξ , which after rescaling would contribute terms to the integral of order $\delta^p \cdot \delta^2$ with $p \geq 1$. Returning to general coordinates, we summarize the conclusion for the local velocity (5.33): For a point y near the curve, if $y = x + bn$, where x is on the curve and n is the normal at x ,

$$\nu v^L = -\frac{\delta^2}{8\pi} \beta \left(\sqrt{\pi} e^{-\beta^2} - 2\pi |\beta| \operatorname{erfc}|\beta| \right) F_\tau \tau + O(\delta^3) \quad (5.43)$$

where $\beta = b/\delta$, τ is tangent at x , and F_τ is the tangential component of F at x .

Finally, we consider the case of an integral over the full periodic domain but with a discontinuity in F at the curve Γ . In the analysis above, if our integral were outside D rather than inside, the y -integral would have been from $-b$ to ∞ rather than $-\infty$ to $-b$. The answer would be the same except for a change of sign. Thus, for an integral with discontinuity across Γ , the result would be the difference of two terms as in (5.43),

$$\nu v^L = \frac{\delta^2}{8\pi} \beta \left(\sqrt{\pi} e^{-\beta^2} - 2\pi |\beta| \operatorname{erfc}|\beta| \right) [F_\tau] \tau + O(\delta^3) \quad (5.44)$$

where $[F_\tau]$ means the outside value minus the inside.

6 An exact solution with elastic force

?? Sign of curvature changed to conform with other sections ?? This is a minor rewrite of earlier note ?? We should do some cutting before submitting

We will shall construct an exact solution in the 2π -periodic domain in which the elastic interface is a moving ellipse. We take the ellipse to be

$$x = a(t) \cos \theta, \quad y = b(t) \sin \theta \quad (6.1)$$

parametrized by θ , so at one time the ellipse is

$$\frac{x^2}{a^2} + \frac{y^2}{b^2} = 1. \quad (6.2)$$

The area must remain constant since the flow is incompressible, and we take $a(t)b(t) = 1$ to preserve the area. To be specific, we take

$$a(t) = 1 + \frac{1}{4} \cos \omega t \quad (6.3)$$

with some frequency ω so that $3/4 \leq a \leq 5/4$ and $4/5 \leq b \leq 4/3$, and the ellipse is well within the square $-\pi/2 \leq x, y \leq \pi/2$. We assume that the points move along rays $\theta = \text{constant}$. Then the velocity of a point on the ellipse is

$$(a' \cos \theta, b' \sin \theta). \quad (6.4)$$

We note for later that $ds/d\theta \equiv \sigma$ is

$$\sigma = \sqrt{a^2 \sin^2 \theta + b^2 \cos^2 \theta} = \sqrt{b^4 x^2 + a^4 y^2} \quad (6.5)$$

where $s = \text{arclength}$. The unit tangent and normal vectors are

$$\tau = (-a^2 y, b^2 x)/\sigma, \quad n = (b^2 x, a^2 y)/\sigma. \quad (6.6)$$

Also $\partial\tau/\partial s = -\sigma^{-3}n$. We have $\partial\tau/\partial s = -\kappa n$ with curvature $\kappa = \sigma^{-3}$.

The next step is to find a velocity field which gives the motion specified for the ellipse. We choose a stream function $\psi^{(0)}$ and then define the velocity as $(\psi_y^{(0)}, -\psi_x^{(0)})$, so that the divergence is zero. Note that $a'/a = -b'/b$ since $ab = 1$. For $-\pi/2 \leq x, y \leq \pi/2$ we define

$$\psi^{(0)} = \frac{a'}{a} xy \quad (6.7)$$

so that

$$v^{(0)} = \left(\frac{a'}{a}x, \frac{b'}{b}y\right) \quad (6.8)$$

in this smaller region, matching the velocity already specified on the curve. Later we extend $\psi^{(0)}$ to $-\pi \leq x, y \leq \pi$ so that it is periodic. We note for later use that $\Delta v^{(0)} = 0$.

We suppose that the equilibrium of the membrane is the circle of radius $1/2$, with total length π , and $\theta = 2\alpha$ or $\alpha = \theta/2$, so that α is a material coordinate.

Then $ds/d\alpha = (ds/d\theta)(d\theta/d\alpha) = 2\sigma$. The force f on the curve is given in terms of τ , n , and $s_\alpha = ds/d\alpha$,

$$f = \partial_s[(s_\alpha - 1)\tau] = 2\partial_s(s_\theta)\tau - (2s_\theta - 1)\kappa n = f_\tau\tau + f_n n \quad (6.9)$$

with

$$f_\tau = 2\partial_s(s_\theta), \quad f_n = -(2s_\theta - 1)\kappa \quad (6.10)$$

and since $\sigma = s_\theta$,

$$f_\tau = 2s_{\theta\theta}/\sigma = 2\sigma^{-2}(a^2 - b^2)xy \quad (6.11)$$

$$f_n = -\sigma^{-3}(2\sigma - 1) = -2\sigma^{-2} + \sigma^{-3}. \quad (6.12)$$

We must choose v and p with the jump conditions (outside minus inside)

$$f = [p]n - \nu \left[\frac{\partial v}{\partial n} \right] \quad (6.13)$$

or, separating tangent and normal components,

$$\left[\frac{\partial v}{\partial n} \right] = -f_\tau \tau, \quad [p] = f_n. \quad (6.14)$$

To create tangential force on the boundary, we will add a term to the velocity inside the ellipse, giving the jump in normal velocity. Since the velocity must be continuous, the new term must be zero on the curve. We again define it through a stream function. We define ρ by

$$\rho^2 = \frac{x^2}{a^2} + \frac{y^2}{b^2} \quad (6.15)$$

so that the ellipse corresponds to $\rho = 1$. Let g be any function near the ellipse. Define

$$\psi^{(1)} = g(\rho^2 - 1)^2, \quad v^{(1)} = (\psi_y^{(1)}, -\psi_x^{(1)}). \quad (6.16)$$

For any choice of g , the velocity will be continuous with a jump in $\partial v/\partial n$ depending on g . We find $\Delta(\rho^2 - 1)^2 = 8\sigma^2$. Since $\psi = 0$ and $\nabla\psi = 0$ on the ellipse we get

$$\frac{\partial v^{(1)}}{\partial n} = -g(\Delta(\rho^2 - 1)^2)\tau = -8\sigma^2 g\tau. \quad (6.17)$$

Looking at f_τ above, we need $-8\sigma^2 g = f_\tau$ on the ellipse, or

$$g = -\frac{1}{4\sigma^4}(a^2 - b^2)\sin\theta\cos\theta = -\sigma^{-4}(a^2 - b^2)\frac{xy}{4ab} \quad (6.18)$$

on the ellipse. We will extend σ positively to the interior $\rho < 1$ and then define, for $\rho < 1$,

$$\psi^{(1)} = -\sigma^{-4}(a^2 - b^2)\frac{xy}{4ab}(\rho^2 - 1)^2 \quad (6.19)$$

Similarly, we define p inside as the extension of $-f_n = \sigma^{-3}(2\sigma - 1)$, with $p = 0$ outside, so that the jump condition for pressure in (6.14) is satisfied. We have now defined the velocity and pressure so that the ellipse moves with the fluid velocity and the jump conditions (6.14) hold.

To extend σ to $\rho < 1$, keeping it positive, we define σ^2 inside as

$$\sigma^2 = 1 + (a^2 - 1)\frac{y^2}{b^2} + (b^2 - 1)\frac{x^2}{a^2}. \quad (6.20)$$

Then $\sigma^2 \rightarrow 1$ as $(x, y) \rightarrow (0, 0)$, and for $\rho = 1$ it is

$$1 + a^2\frac{y^2}{b^2} + b^2\frac{x^2}{a^2} - 1 \quad (6.21)$$

which agrees with (6.5) since $ab = 1$. We check it is strictly positive:

$$\sigma^2 = 1 - \rho^2 + a^2\frac{y^2}{b^2} + b^2\frac{x^2}{a^2}. \quad (6.22)$$

Choose $c_0 > 0$ so that $a, b \geq c_0$ at each time. (For our example, $c_0 = 3/4$.) Then

$$\sigma^2 \geq 1 - \rho^2 + c_0\rho^2 = 1 - (1 - c_0)\rho^2 \geq c_0 \quad (6.23)$$

for $\rho^2 \leq 1$, as desired.

We need third derivatives of $\psi^{(1)}$, since $v^{(1)} = (\psi_y^{(1)}, -\psi_x^{(1)})$ and the body force depends on $\Delta v^{(1)}$. To record various derivatives, we write

$$\psi^{(1)} = C_0xyQR, \quad C_0 = (b^2 - a^2)/(4ab), \quad (6.24)$$

$$Q = \sigma^{-4}, \quad R = (\rho^2 - 1)^2 \quad (6.25)$$

with σ extended to $\rho \leq 1$ as in (6.20),(6.22). For convenience write

$$\rho^2 = b^2x^2 + a^2y^2, \quad \sigma^2 = 1 + b^2(b^2 - 1)x^2 + a^2(a^2 - 1)y^2 \quad (6.26)$$

or

$$\sigma^2 = 1 + Bx^2 + Ay^2, \quad B = b^2(b^2 - 1), \quad A = a^2(a^2 - 1) \quad (6.27)$$

Then

$$R_x = 4(\rho^2 - 1)b^2x, \quad R_y = 4(\rho^2 - 1)a^2y, \quad R_{xy} = 8xy \quad (6.28)$$

$$R_{xx} = 8b^4x^2 + 4(\rho^2 - 1)b^2, \quad R_{yy} = 8a^4y^2 + 4(\rho^2 - 1)a^2, \quad (6.29)$$

$$\Delta R_x = 8x(1 + 3b^4), \quad \Delta R_y = 8y(1 + 3a^4) \quad (6.30)$$

$$Q_x = -4\sigma^{-6}Bx, \quad Q_y = -4\sigma^{-6}Ay, \quad Q_{xy} = 24\sigma^{-8}ABxy \quad (6.31)$$

$$Q_{xx} = 4\sigma^{-8}B(5Bx^2 - 1 - Ay^2), \quad Q_{yy} = 4\sigma^{-8}A(5Ay^2 - 1 - Bx^2), \quad (6.32)$$

$$\Delta Q_x = 24\sigma^{-10}Bx(3B - 5B^2x^2 + 3ABy^2 + A + ABx^2 - 7A^2y^2) \quad (6.33)$$

$$\Delta Q_y = 24\sigma^{-10}Ay(3A - 5A^2y^2 + 3ABx^2 + B + ABY^2 - 7B^2x^2) \quad (6.34)$$

Using derivatives of R and Q we can write

$$v_1^{(1)} = (\psi_y^{(1)} = C_0xQR + C_0xy(Q_yR + QR_y) \quad (6.35)$$

$$v_2^{(1)} = -(\psi_x^{(1)} = -C_0yQR - C_0xy(Q_xR + QR_x) \quad (6.36)$$

$$\begin{aligned} \Delta v_1^{(1)}/C_0 = \Delta \psi_y^{(1)}/C_0 = & 2QR_x + 2Q_xR \\ & + 2y(Q_{xy}R + Q_xR_y + QR_{xy} + Q_yR_x) \\ & + x(6Q_yR_y + 3QR_{yy} + 3Q_{yy}R + Q_{xx}R + QR_{xx} + 2Q_xR_x) \\ & + xy((\Delta Q_y)R + 3Q_{yy}R_y + 3Q_yR_{yy} + Q\Delta R_y \\ & + Q_{xx}R_y + 2Q_{xy}R_x + 2Q_xR_{xy} + Q_yR_{xx}) \end{aligned} \quad (6.37)$$

$$\begin{aligned} -\Delta v_2^{(1)}/C_0 = \Delta \psi_x^{(1)}/C_0 = & 2QR_y + 2Q_yR \\ & + 2x(Q_{xy}R + Q_yR_x + QR_{xy} + Q_xR_y) \\ & + y(6Q_xR_x + 3QR_{xx} + 3Q_{xx}R + Q_{yy}R + QR_{yy} + 2Q_yR_y) \\ & + xy((\Delta Q_x)R + 3Q_{xx}R_x + 3Q_xR_{xx} + Q\Delta R_x \\ & + Q_{yy}R_x + 2Q_{xy}R_y + 2Q_yR_{xy} + Q_xR_{yy}) \end{aligned} \quad (6.38)$$

With these pieces in place, we can write explicitly the velocity v , pressure p , and body forces, inside and outside the ellipse. Inside we use (6.8), (6.35), (6.36) to define

$$v = v^{(0)} + v^{(1)}, \quad \rho < 1 \quad (6.39)$$

and p as stated before, using the extended σ in (6.20),

$$p = \sigma^{-3}(2\sigma - 1), \quad \rho < 1 \quad (6.40)$$

so that

$$\nabla p = \sigma^{-5}(3 - 4\sigma)(Bx, Ay), \quad \rho < 1. \quad (6.41)$$

To define v outside the ellipse, we use a periodic extension of $\zeta(x) = x$ for $|x| \leq \pi/2$, extended to $|x| \leq \pi$, as defined below. Outside the ellipse we define, in place of (6.7),

$$\psi^{(0)}(x, y) = \frac{a'}{a}\zeta(x)\zeta(y) \quad (6.42)$$

so that the outside velocity is

$$v = (\psi_y^{(0)}, -\psi_x^{(0)}) = \frac{a'}{a}(\zeta(x)\zeta'(y), -\zeta'(x)\zeta(y)), \quad \rho > 1. \quad (6.43)$$

We take the pressure to be zero outside,

$$p = 0, \quad \rho > 1. \quad (6.44)$$

To use this example as a test problem, we need to give the nonhomogeneous terms, or body force, as well as the force on the boundary, in order to compute v and p , and compare with the exact ones above. The Stokes equations have the form (1.1), (1.2) with force $F = f\delta_\Gamma + F_b$ where F_b is the body force (interior and exterior) and $f\delta_\Gamma$ is the force on the boundary. The boundary force is $f = f_n n + f_\tau \tau$, with n, τ given by (6.6) and f_n, f_τ given by (6.10) or (6.11),(6.12). As for the body force F_b , we have with the choices above,

$$F_b = -\nu \Delta v^{(1)} + \nabla p, \quad \rho < 1 \quad (6.45)$$

and

$$F_b = -\nu(\Delta\psi_y^{(0)}, -\Delta\psi_x^{(0)}). \quad \rho > 1. \quad (6.46)$$

Inside, the components of F_b are given by (6.37),(6.38),(6.41), taking into account the factors C_0 and $-\nu$.) Outside they are

$$F_{b1} = -\nu \frac{a'}{a} (\zeta''(x)\zeta'(y) + \zeta(x)\zeta'''(y)), \quad \rho > 1 \quad (6.47)$$

$$F_{b2} = \nu \frac{a'}{a} (\zeta'''(x)\zeta(y) + \zeta'(x)\zeta''(y)), \quad \rho > 1. \quad (6.48)$$

Finally we give the definition of ζ . We first construct an odd polynomial $q(x)$ on $[-\pi/2, \pi/2]$, so that after translation ζ will be odd about $x = \pm\pi$. We specify $q'(\pi/2) = 1$; $q''(\pi/2) = 0$; $q'''(\pi/2) = 0$. With

$$q(x) = c_1 x + c_2 x^3 + c_3 x^5 + c_4 x^7 \quad (6.49)$$

we get

$$c_1 = -\frac{27}{8}, \quad c_2 = \frac{35}{2\pi^2}, \quad c_3 = -\frac{42}{\pi^4}, \quad c_4 = \frac{40}{\pi^6}. \quad (6.50)$$

Now define

$$\zeta(x) = x, \quad -\pi/2 \leq x \leq \pi/2 \quad (6.51)$$

$$\zeta(x) = q(x - \pi), \quad \pi/2 \leq x \leq \pi \quad (6.52)$$

$$\zeta(x) = q(x + \pi), \quad -\pi \leq x \leq -\pi/2 \quad (6.53)$$

We have defined ζ so that ζ''' is continuous but not differentiable at $x = \pm\pi/2$. Thus the body force F_b has the same property. For reference here are the derivatives of p :

$$q'(x) = c_1 + 3c_2 x^2 + 5c_3 x^4 + 7c_4 x^6 \quad (6.54)$$

$$q''(x) = 6c_2 x + 20c_3 x^3 + 42c_4 x^5 \quad (6.55)$$

$$q'''(x) = 6c_2 + 60c_3 x^2 + 210c_4 x^4 \quad (6.56)$$

The maximum of $|q'''|$ is about 11, occurring near $x = 0$ (which gets converted to $x = \pm\pi$). In between it peaks at about -8 . The maximum of $|q|$ itself is about 2. But the maximum of q'''' is about 50.

7 Numerical results

8 Future Directions

?? How's that for the title? ?? start by saying we have a new method ?? and it works great?

The algorithm used in this work extends directly to three dimensions, although more work is required. If the force on a moving surface is determined by stretching of area, the description of the evolution in Sec. 2 applies directly. The Stokes velocity resulting from the interfacial force is a single layer potential on the surface with $1/r$ singularity. The Ewald splitting applies to the fundamental solution, and the treatment of the Fourier part of the integral is the same [29]. The local part can be approximated as in Sec. 5; a method of this type for surface layer potentials for the Laplacian was developed in [3] and a general approach given in [23]. A code has already been written for the semi-Lagrangian contouring method in three dimensions. ?? J, do you want a citation for the above? Or delete this?

We have assumed that the viscosity is the same on both sides of the interface. Boundary integral methods have been used for Stokes flow with different viscosities (e.g. see [22,21]). The calculation of the velocity determined by the force on the moving boundary requires the solution of an integral equation on the boundary as a preliminary step (e.g., see [22,21,1]). The present method should extend to the case of differing viscosities in this way.

The Stokes equations (1.1) describe fluid flow only for very low Reynolds number. More generally (1.1) should be replaced by the Navier-Stokes equations

$$v_t + v \cdot \nabla v + \nabla p = \nu \Delta v + f \delta_\Gamma, \quad \nabla \cdot v = 0. \quad (8.1)$$

We expect the present method can be extended to Navier-Stokes flow with an elastic interface. One way to proceed begins with the observation that the jump conditions (1.6) are the same in the two cases. At each time we can write the Navier-Stokes velocity v of (8.1) as a sum $v = v^s + v^r$ where v^s is the Stokes velocity, the solution of (1.1). Then v^r is C^1 at the interface; the jump in the normal derivative has been removed. The evolution equation for the regular part v^r is similar to (8.1), without the interfacial force, but with a forcing term determined by v^s . It should be possible to solve for v^r accurately on a

regular grid. With this additional step the procedure could be an extension of the method presented here for Stokes flow.

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?? John check wording and your grant numbers, copied from your box paper.

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References

- [1] J. T. Beale and A. Layton, On the accuracy of finite difference methods for elliptic problems with interfaces, *Commun. Appl. Math. Comput. Sci.* 1 (2006), 91-119 (www.camcos.org).
- [2] J. T. Beale and M.-C. Lai, A method for computing nearly singular integrals, *SIAM J. Numer. Anal.* 38 (2001), 1902-25.
- [3] J. T. Beale, A grid-based boundary integral method for elliptic problems in three dimensions, *SIAM J. Numer. Anal.* 42 (2004), 599-620.
- [4] G. Biros, L. Ying, and D. Zorin, A fast solver for the Stokes equations with distributed forces in complex geometries, *J. Comput. Phys.* 193 (2004), 317-348.
- [5] G. Biros, L. Ying, and D. Zorin, An embedded boundary integral solver for the unsteady incompressible Navier-Stokes equations, submitted, 2004.
- [6] R. Cortez, The method of regularized Stokeslets, *SIAM J. Sci. Comput.* 23 (2001), 1204-1225.
- [7] R. Cortez and M. Minion, The blob projection method for immersed boundary problems, *J. Comput. Phys.* 161 (2000), 428-453.
- [8] G.-H. Cottet and E. Maitre, A level-set formulation of immersed boundary methods for fluid-structure interaction problems, *C. R. Math. Acad. Sci. Paris* 338 (2004), no. 7, 581-586.
- [9] G.-H. Cottet and E. Maitre, A level-set method for fluid-structure interactions with immersed surfaces, *Mathematical Models and Methods in the Applied Sciences* 16 (2006), 415-438.

- [10] L. Greengard and J. Strain, *Commun. Pure Appl Math.* 43 (1990), 949-63.
- [11] B. Griffith and C. Peskin, On the order of accuracy of the immersed boundary method: Higher order convergence rates for sufficiently smooth problems, *J. Comput. Phys.* 208 (2005), 75–105.
- [12] D. D. Joseph and Y. Y. Renardy, *Fundamentals of Two-Fluid Dynamics, Part I: Mathematical Theory and Applications*, Springer, New York, 1993.
- [13] M. Kropinski, An efficient numerical method for studying interfacial motion in two-dimensional creeping flows, *J. Comput. Phys.* 171 (2001), 479-508.
- [14] L. G. Leal, *Laminar Flow and Convective Transport Processes*, Butterworth-Heinemann, Boston, 1992.
- [15] L. Lee and R. LeVeque, An immersed interface method for incompressible Navier-Stokes equations, *SIAM J. Sci. Comput.* 25 (2003), 832–856.
- [16] R. J. LeVeque and Z. Li, Immersed interface methods for Stokes flow with elastic boundaries or surface tension, *SIAM J. Sci. Comput.* 18 (1997), 709–735.
- [17] Z. Li and M.-C. Lai, The immersed interface method for the Navier-Stokes equations with singular forces, *J. Comput. Phys.* 171 (2001), 822-42.
- [18] A. Mayo and C. Peskin, An implicit numerical method for fluid dynamics problems with immersed elastic boundaries, *Contemp. Math.* 141 (1993), 261-77.
- [19] C. Peskin, The immersed boundary method, *Acta Numer.* 11 (2002), 479–517.
- [20] C. Peskin and B. Printz, Improved volume conservation in the computation of flows with immersed elastic boundaries, *J. Comput. Phys.* 105 (1993), 33–46.
- [21] C. Pozrikidis, Interfacial Dynamics for Stokes Flow, *J. Comput. Phys.* 169 (2001), 250–301.
- [22] C. Pozrikidis, *Boundary Integral and Singularity Methods for Linearized Viscous Flow*, Cambridge Univ. Press, Cambridge, 1992.
- [23] J. Strain, Locally-corrected spectral methods and overdetermined elliptic systems (preprint).
- [24] J. Strain, A fast semi-Lagrangian contouring method for moving interfaces, *J. Comput. Phys.* 170 (2001), 373–394.
- [25] J. Strain, A fast modular semi-Lagrangian method for moving interfaces, *J. Comput. Phys.* 161 (2000), 512–536.
- [26] J. Strain, Fast tree-based redistancing for level set computations, *J. Comput. Phys.* 152 (1999), 664–686.
- [27] J. Strain, Tree methods for moving interfaces. *J. Comput. Phys.* 151 (1999), 616–648.

- [28] J. Strain, Semi-Lagrangian methods for level set equations, *J. Comput. Phys.* 151 (1999), 498–533.
- [29] J. Strain, Fast potential theory. II. Layer potentials and discrete sums, *J. Comput. Phys.* 99 (1992), 251–270.
- [30] A.-K. Tornberg and M. Shelley, Simulating the dynamics and interactions of flexible fibers in Stokes flows, *J. Comput. Phys.* 196 (2004), 8-40.
- [31] C. Tu and C. Peskin, Stability and instability in the computation of flows with moving immersed boundaries: a comparison of three methods, *SIAM J. Sci. Statist. Comput.* 13 (1992), 1361–1376.
- [32] H.-K. Zhao, T. Chan, B. Merriman, and S. Osher, A variational level set approach to multiphase motion, *J. Comput. Phys.* 127 (1996), 179–95.