Boundary Integral Methods for Interfaces

These are some very informal notes corresponding to my talk on Wed. Oct. 1 including some things I didn't mention there. I don't guarantee that all signs are correct etc. You can ask me about more specific references if you want. Other people in the group will know more about some things. My recent papers can be found at my web site, www.math.duke.edu/faculty/beale.

What do integrals have to do with interfaces? Let's start with harmonic functions since they are familiar. For the Laplacian Δ we have the fundamental solution $G(x)$ so that $\Delta G = \delta$. In $\mathbb{R}^2$, $G(x) = (1/2\pi)\log r$ and in $\mathbb{R}^3$, $G(x) = -1/(4\pi r)$, where $r = |x|$. If Γ is a closed surface in 3D or a closed curve in 2D, we define a double layer potential as

$$u(x) = \int_\Gamma \frac{\partial G(x-y)}{\partial n(y)} f(y)\, dS(y)$$

where f is some given function on Γ and we use the outward normal n. For x inside or outside of Γ, $\Delta u = 0$, but u has a jump at Γ:

$$u(x\pm) = \mp\tfrac{1}{2} f(x) + \int_\Gamma \frac{\partial G(x-y)}{\partial n(y)} f(y)\, dS(y)$$

Thus if we are given f on Γ and we want to find u with jump $(u+) - (u-) = -f$, we could define u in this way. The single layer potential is continuous at Γ, but the normal derivative has a jump. Thus if jumps are specified in u and its normal derivative, we can find a harmonic function with the given jumps by adding two terms. This is all very classical and in many pde books.

Boundary integrals have been used for a long time for computing fluid flow with moving boundaries. To say how, let's start with the Navier-Stokes equations

$$\rho(v_t + v\cdot\nabla v) = -\nabla p + \mu\Delta v + F$$

$$\nabla\cdot v = 0$$

Here v is velocity, p is pressure, ρ is density, μ is viscosity. I'll assume ρ, μ constant here. (Of course we are interested in more general problems.) If the equations are nondimensionalized then μ is one over the Reynolds number Re. Boundary integrals are useful at the two extremes, viscosity zero or viscosity dominant.

Stokes flow, or creeping flow, is the special case where we neglect the material derivative above and have

$$-\nabla p + \mu\Delta v + F = 0\,, \qquad \nabla\cdot v = 0$$

The interface still moves with the fluid velocity, even though the problem for velocity/pressure has no time deriv. This model is appropriate at small scales, as in many biology problems; Lisa Fauci talked about such things at the workshop. Charles Peskin's immersed boundary method (not an integral method) has been used for such problems. The interface may exert a force on the fluid in which case F above could be $F = f\delta_\Gamma$ where here the δ restricts to the interface. The resulting equation amounts to having $F = 0$ off the interface but jump conditions. They are naturally expressed in terms of the stress $\sigma_{ij} = -\delta_{ij} p + \mu(v_{i,j} + v_{j,i})$. Then the condition is that the normal stress jumps by f,

$$\sum_j [\sigma_{ij}] n_j = -f_j$$

where $[\cdot]$ means the jump.

The Stokes equations are an elliptic pde system. Let's set $\mu = 1$. The solution of

$$-\Delta v + \nabla p = F\,, \qquad \nabla \cdot v = 0$$

in free space is

$$v_i = \sum_j S_{ij} \star F_j$$

where S_{ij} is the fundamental solution or Stokeslet, in 2D

$$4\pi S_{ij} = -\delta_{ij} \log r + x_i x_j / r^2$$

and in 3D

$$8\pi S_{ij} = \delta_{ij}/r + x_i x_j / r^3$$

Think of this as like G for the Laplacian but more complicated. The sol'n of the Stokes problem with $F = f\delta_\Gamma$ is a surface integral like the single layer potential for the Laplacian.

The simplest case of the force f is constant surface tension, f proportional to κn, where κ is mean curvature. For this case boundary integral methods have long been used to compute the motion of a drop of one fluid in another. These started with Acrivos. See especially the books of Pozrikidis especially his "Boundary Integrals and Singularity Methods" for the theory, elsewhere for numerics. There was a nice review artice by Howard Stone in the Ann. Rev. of Fluid Mech. 1994. Maybe there's a more recent one. There is nice work by Zinchenko probably in J. Comput. Phys. (JCP) with 3D drops which shows the "state of the art". In all this work it is important that the velocity is computed only on the interface. For Stokes flow, unlike NS, it is not necessary to find it off the interface to move the interface. To find the velocity off the interface we encounter "nearly singular" integrals, mentioned below.

Such methods are used much more generally. The interface may exert an elastic force, as in biology problems. There is interesting work by Cortez and Fauci at Tulane and by M. Shelley and A-K Tornberg (separately and together) at the Courant Inst, NYU. John Strain and I have a recent paper about this, submitted to JCP.

At the other end, neglecting viscosity, boundary integrals are often used for potential flow, i.e, vorticity zero or concentrated on interfaces. Applications include vortex sheets and water waves. Methods for water waves are practical in 2D and have been developed in 3D. There was a survey article by Tsai and Yue in Ann Rev Fl Mech a few years back. Also see work of F. Dias among others. Some of my work has been about analysis of such methods for water waves.

Boundary integral methods are often used for electromagnetic scattering. The important equation is the Helmholtz equation

$$\Delta u + k^2 u = 0$$

For many realistic cases k is large, introducing difficulties we do not consider here. The work of Oscar Bruno and his group at Caltech is notable.

We will comment on various issues of implementing the methods. Naturally 3D is harder than 2D, and in several ways. In principle the way the interface is moved is independent of the integral representation, but usually in integral methods markers are moved, i.e. the interface is tracked. This is not hard to implement in 2D. If the markers are material, or Lagrangian, moving with the fluid velocity, then they may not be well placed after a while. Remeshing can be used; it might introduce significant errors, but not necessarily. The placement of the markers can be improved by choosing a tangential velocity which doesn't affect the surface (or curve). This was done with success in the method of Hou, Lowengrub and Shelley "Removing the Stiffness..."

How to represent a surface in 3D is not simple. There is a well developed field of boundary element methods in which the surface is triangulated and singular integrals are computed in the elements. This has analogies with the finite element method but has extra problems. It is practical in in steady problems, but probably for moving boundaries we don't want to make so much effort for one boundary. A thorough treatment of this method can be found in the book of Hackbush. Also see work of Schwab, and probably many others. For other ways of representing interfaces see work of Cristini especially. My preference is to use overlapping coordinate charts and a partition of unity; see my paper "A Grid-Based..." Of course this is more work. That approach is also used in O. Bruno's work and work of Biros, Lexing Ying, and Zorin.

How to compute the singular integral? In 2D the exact singularity has limited form, usually log or $1/x$, and there are definitive rules for both. If we want the velocity at grid points near the curve, but not on it, we have a nearly singular integral, which is generally harder. I would regularize and then discretize; see my paper with M.C. Lai, "A Method for Computing Nearly Singular Integrals". That approach extends to 3D, as in my other paper already mentioned. The exact singularities in 3D generally have the form 1/r. That is often removed by introducing polar coordinates; see work of Schwab as well as Bruno and coworkers. The regularization I would use makes special coordinates unnecessary.

Regularization is related to Ewald summation, which splits the fundamental solution into a local, singular part and a smooth part. It is especially useful for periodic problems. John Strain has a good point of view on this. See his paper "Fast Potential Theory II" or a recent paper he and I wrote on Stokes flow with an elastic interface. In our paper we compute the velocity at grid points as well as on the interface; our approach is meant to be "upwardly compatible" with Navier-Stokes.

Some disadvantages and what can be done about them: If the integral for the velocity on a surface has N points there are in principle N^2 operations and this could be prohibitive. Practical methods will depend on fast summation methods. The best known is that of L. Greengard and V. Rokhlin. There are interesting variants, e.g. the kernel-free method of Biros, Ying and Zorin. They and Bruno replace sources with equivalent sources, but Bruno uses FFT's. For the boundary integral method, basically we need to know the fundamental solution, but that is not strictly so. We mentioned periodic cases above. Strain (and maybe others?) have tried preconditioning variable coeff't problems with the constant coeff't case. Wenjun Ying in a recent paper treated general integral problems, with variable coeff'ts, to an interface problem treated by the immersed interface method. Topological changes are not natural with integral methods.