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Immersed Interface Methods
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1 Background

Cartesian grid methods encompass a wide variety of techniques used to solve partial differential equations in more than one space dimension on uniform Cartesian grids (perhaps adaptively refined) even when the underlying geometry is complex and not aligned with the grid. LeVeque's work in this area extends back a decade and initially concerned method for compressible gas dynamics, including much joint work with Marsha Berger [8], [9], [10], [11], [35], [36], [37]. Many other Cartesian grid methods have been developed for a wide variety of different problems, and interest in such methods appears to be growing, especially in three dimensions where the generation of good body-fitted grids can often be difficult. Problems where the boundary or some interface within the region is *moving* are also more easily modeled on an underlying simple grid rather than on moving grids. A sample of Cartesian grid methods includes [4], [23], [24], [30], [31], [53], [51], [54], [52], [55], [61], [63], [67], [66], [69].

Our groups work on *Immersed Interface Methods* (often abbreviated IIM below) was originally motivated by the desire to understand and improve the "Immersed Boundary Method", developed by Charles Peskin to solve incompressible Navier-Stokes equations in complicated geometries with moving elastic boundaries, specifically for studying blood flow in the heart and the functioning of artificial heart valves[56], [57],[58],[59],[60].

Peskin's idea was to view the entire heart as being immersed in a Cartesian box of fluid (a square in the original 2D model or a cube in his current 3D model). The incompressible Navier-Stokes equations are solved on a uniform Cartesian grid in this box and the outer heart wall (as well as interior walls separating chambers, valve leaflets, etc.) are viewed as being immersed within the fluid. These structures are modeled by a separate Lagrangian set of grid points that move with the local fluid velocity in order to impose the requirement that no fluid can flow through the wall.

In each time step, the Navier-Stokes equations are solved on the uniform grid to determine

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the fluid velocities at each of these grid points. These velocities are then interpolated to the immersed boundary points to determine its motion. Of course the boundary must also have an effect on the fluid, and this is modeled by adding a forcing term to the Navier-Stokes equations to represent the force exerted on the fluid by the immersed boundary. This is a singular (delta function) force with support only along the boundary. The strength of this force depends on the nature and position of the boundary. The force is spread to the neighboring uniform grid points via a *discrete delta function*, an ordinary function with small support and total mass 1.

This approach is remarkably effective and has been used on a wide variety of problems. Applications include aquatic locomotion [25], blood platelet aggregation [27] [28], [29], and wave motion in the cochlea (by LeVeque's student Richard Beyer) [16], [17]. Similar approaches have also been used outside of biophysics, e.g., to sedimentation [64] and bubble dynamics [66], [67]. However, the method is at most first order accurate due to the way the singular force is smeared out over an $O(h)$ region.

2 Immersed Interface Methods

Attempts to achieve better accuracy with a Cartesian grid method of this form gave rise to the Immersed Interface Method (IIM). LeVeque and Beyer [16], [18] first analyzed one-dimensional problems and found that a discrete delta function approach can give second order accuracy in many cases if an appropriate delta function d_h is used. However, in two dimensions it does not appear possible to achieve second order accuracy, even on simple model problems, simply by choosing an appropriate discrete delta function.

However, LeVeque's student Zhilin Li (now at UCLA) discovered that the analytical techniques used by Beyer and LeVeque to prove second order accuracy could be used directly to develop second order methods in more dimensions, without introducing discrete delta functions. The idea is to use Taylor series expansions to derive second order accurate finite difference methods following standard analysis of the local truncation error, but taking into account the nonsmoothness of the solution that is induced by the singularity at the interface in doing these expansions.

Consider, for example, the problem of discretizing u_{xx} near a point $x = \alpha$ where the function and derivatives have known jumps $[u] = C_0$, $[u_x] = C_1$, etc., as in the figure:

Figure 1: Discontinuity at $x = \alpha$ between grid points.

The standard centered approximation $(U_{j-1} - 2U_j + U_{j+1})/h^2$ would not work. But we can

expand in Taylor series as

$$u(x_{j-1}) = u^- + (x_{j-1} - \alpha)u_x^- + \frac{1}{2}(x_{j-1} - \alpha)^2 u_{xx}^- + \dots \quad (1)$$

$$u(x_j) = u^- + (x_j - \alpha)u_x^- + \frac{1}{2}(x_j - \alpha)^2 u_{xx}^- + \dots \quad (2)$$

$$u(x_{j+1}) = u^+ + (x_{j+1} - \alpha)u_x^+ + \frac{1}{2}(x_{j+1} - \alpha)^2 u_{xx}^+ + \dots \quad (3)$$

where $+$ and $-$ superscripts indicate limiting values as we approach α from the right and left. Using the jump conditions we can rewrite (3) as

$$u(x_{j+1}) = (u^- + C_0) + (x_{j+1} - \alpha)(u_x^- + C_1) + \frac{1}{2}(x_{j+1} - \alpha)^2 (u_{xx}^- + C_2) + \dots \quad (4)$$

Then from (1), (2), (4) we find that

$$\begin{aligned} u_{xx}(x_j) &= u_{xx}^- + O(h) \\ &= \frac{1}{h^2} \left(U_{j-1} - 2U_j + U_{j+1} - C_0 - (x_{j+1} - \alpha)C_1 + \frac{1}{2}(x_{j+1} - \alpha)^2 C_2 \right) + O(h). \end{aligned} \quad (5)$$

This shows how to correct the standard centered approximation to get a first order accurate approximation to u_{xx} , which is typically enough to maintain global second order accuracy[42]. Note that for a problem with a delta function source we typically have $C_0 = C_2 = 0$ and C_1 is the strength of the delta source, and the correction term in (5) is $C_1(x_{j+1} - \alpha)/h^2$, which is a discrete delta function in the form of a hat function with width h centered at α and evaluated at x_j , showing the connection to the discrete delta function approach in this simple case. In two dimensions the Taylor series expansion approach still works but does not reduce to a simple discrete delta function.

Another nice feature of this approach is that it is easily extended to problems with discontinuous coefficients as well as singular forces. For example, the heat equation $u_t = (\beta(x)u_x)_x$ where $\beta(x)$ is discontinuous at some point α will yield a discontinuity in u_x at the same point. Again we know the jump in u_x , since it can be shown that βu_x is continuous. In this case a three-point approximation to $(\beta u_x)_x$ of the form

$$\gamma_{1,j}U_{j-1} + \gamma_{2,j}U_j + \gamma_{3,j}U_{j+1} \approx (\beta u_x)_x \text{ at } x_j$$

can be devised[42] (perhaps with correction terms as above if there are also singular sources in the equation). Jumps in the solution u can also be handled as easily as jumps in u_x , which corresponds, for example, to having a dipole source of the form $\delta'(x - \alpha)$ in the equation.

3 Elliptic equations

The original work of Li[45] and LeVeque and Li[42] was for elliptic equations in two dimensions of the form

$$(\beta u_x)_x + (\beta u_y)_y + \kappa u = f \quad (6)$$

where β may be discontinuous across some interface Γ (a smooth curve) and f is smooth away from Γ . This equation is coupled with jump conditions of the form

$$[u] = v(s), \quad [\beta u_n] = w(s)$$

where s parameterizes the interface and u_n is the derivative of u in the direction normal to Γ . The functions v and w can be interpreted as the strength of a double layer and single layer singularity in the forcing term f . If β is continuous then the standard 5-point stencil is used to discretize the left hand side of (6) and the IIM is used to determine the correct right hand side. If β is discontinuous then a 6-point stencil is used for points near the interface. The value at each grid point is expanded in a Taylor series around some point (x^*, y^*) on Γ . The jump conditions at (x^*, y^*) are then used to reduce these expansions to a linear system of 6 equations for the 6 coefficients in the difference stencil. (For details see [42].) This approach is generally quite effective and yields second order accurate solutions uniformly at all grid points, even when the solution is discontinuous. Figure 2 shows one example.

Experience has shown that this approach is not completely robust, however. Some care must be used in picking the sixth point, and occasionally bad stencils are generated. Recently Li[46] has developed a new approach based on dividing (6) by β , which yields

$$u_{xx} + u_{yy} + \frac{1}{\beta}(\beta_x u_x + \beta_y u_y) = f/\beta. \quad (7)$$

So far he has considered only the case of piecewise constant β , in which case this reduces to $u_{xx} + u_{yy} = f/\beta$. Now the standard 5-point stencil can always be used (with fast Poisson solvers) and the discontinuity is moved to the right hand side, where it is easier to handle. The problem is that the jump condition known for the original problem (6) are typically $[u]$ and $[\beta u_n]$. Solving (7) with the IIM requires knowing $[u]$ and $[u_n]$. Li views the jumps in u_n at some M points along the interface as unknowns, to be determined by the constraint that after solving the equation (7), the resulting jumps in βu_n should match the known values. This system of equations is solved using GMRES[62]. Although this requires solving (7) several times as we iterate, it is possible to use fast Poisson solvers, which makes this a competitive method.

For the case of varying β , where the lower order derivatives also appear in (7), Li and Adams are collaborating to use the multigrid method described in Section 4 to solve (7).

Li has also worked out the IIM for three space dimensions, as presented in [48]. A three-dimensional version has also been developed by Jim Keener at the University of Utah to solve electrostatics problems in the heart (personal communication).

4 Multigrid

Adams has developed a full multigrid algorithm to solve the elliptic equation discussed in the last section based on the 6-point stencil. This work was reported at the recent Copper Mountain Conference on multigrid Methods[2]. The scheme uses the IIM to define coarser grid problems, and a modified bilinear interpolation scheme was developed to more accurately move coarse information to a finer grid by taking into account the location of the interface and the jump information there.

The method has been very successful in producing solutions to many problems that include very large jumps in β , (say $10^5:1$), in only one FMG cycle with 4 pre and 4 post rowwise Gauss-Seidel smoothing steps (current results are better than those reported in [2]) and will be reported in [1]. This method was used to calculate the stream function shown in Figure 6 in the presence of multiple interfaces.

In section 2.1, proposed changes to improve the above method as well as proposed changes to apply the above method to the IIM equations (7) will be discussed.

5 Domain embedding for elliptic equations in irregular regions

Adams and her student, Zhiyun Yang, have been using the IIM method to solve elliptic problems where either Dirichlet or Neumann data is given on some irregular region. For these problems, the domain is embedded in a Cartesian grid as described earlier, but now, only one of the jumps in (6) is usually known. The boundary data on the irregular interface is then used to develop a constraint equation involving both the known and unknown jump. This is done using immersed interface ideas to get an accurate constraint equation which leads to a Schur complement system to solve for the unknown jump. Our experience shows this Schur complement system is well-conditioned and can be satisfactorially solved with GMRES[62]. The last step is to apply the IIM method with both jumps known to generate the solution for the variable of interest. We have successfully used this technique to solve for flow around multiple solid objects with good results (Figure 3).

6 ADI for heat equation

Li developed an ADI iteration for solving the heat equation $u_t = u_{xx} + u_{yy} + f$ with singular f . This allows one to solve a sequence of one-dimensional problems involving only tridiagonal matrices in order to advance the solution by one time step. This efficient implicit method is stable and maintains second order accuracy. Anita Mayo had previously developed a very similar ADI method and a joint paper was written[50].

7 Stefan problems

Solidification or melting problems give rise to a Stefan problem. The heat equation with discontinuous coefficients and a singular source term (latent heat release) at the interface must be solved, and additionally the interface must be moved. This gives new difficulties since the time derivative is discontinuous when the interface crosses a grid point. This was initially studied in one dimension by Beyer and LeVeque[18] and in Li[45]. This has been taken further in one dimension by Li[47]. In particular a problem in glaciology has been studied in collaboration between Li and David McTigue in the UW Geology Department, and this work is continuing. Multidimensional Stefan problems will be studied in the future.

8 Stokes flow

The IIM for elliptic equations has been used to develop a method for Stokes flow (zero Reynolds number limit) with immersed elastic interfaces (see Figure 4) or free surfaces as in bubble dynamics. The elastic force or surface tension force gives a singular force along the interface. The two-dimensional Stokes equations with periodic boundary conditions can be reduced to a sequence of 3 Poisson problems, one for the pressure, followed by one for each component of velocity. The pressure is discontinuous across the interface and all three variables have discontinuities in their derivatives there. For the case of an elastic boundary, a test problem

studied by Tu and Peskin[65], comparisons show that our approach gives second order accuracy whereas the discrete delta function approach (immersed boundary method) used in [65] is first order accurate (Figure 4). An efficient fully implicit approach has been developed to avoid the stiffness inherent in this moving interface problem (the primary issue studied in [65]). The method developed, which uses a quasi-Newton method to solve an implicit system of equations for the new location of the interface, could also be used in connection with the classical immersed boundary method. Some other insights gained from this work should also be useful more generally. This work was introduced in Li's thesis[45] and taken further to also study bubble dynamics in [49], [41]. Extension to include the inertial time-derivative term in the Stokes equations is being studied by LeVeque and Li and is related to the solution of heat equations with discontinuous coefficients mentioned above in Section 6.

9 Nonlinear equations

The full Navier-Stokes equations also include nonlinear terms, which introduce new difficulties for two reasons. First it may not be as easy to determine the proper jump conditions from the differential equation or known data, and second it may be more difficult to incorporate these jump conditions into a high order accurate finite difference method. Some one-dimensional model problems have already been studied and progress is being made, both by Li[47] and by Wiegmann and Bube [70]. Ph.D. student Andreas Wiegmann and Bube have been studying the IIM for nonlinear equations with convection nonlinearities of the form $u \cdot \nabla u$ which arise from the total derivative in equations of fluid dynamics. In [70], they have considered both the steady-state and time-dependent Burger's equation with discontinuous viscosity; the spatial derivative terms are of the form $(\beta(x)u_x)_x + uu_x$. The key ansatz which makes the IIM tractable for these nonlinear equations is to look for difference approximations for the spatial derivatives of the form

$$\gamma_{i1}U_{i-1} + \gamma_{i2}U_i + \gamma_{i3}U_{i+1} + U_i(\gamma_{i4}U_{i-1} + \gamma_{i5}U_i + \gamma_{i6}U_{i+1})$$

at the irregular grid points near a jump in $\beta(x)$. This ansatz leads to a *linear* system to recover the coefficients γ_{ij} of the difference scheme at each irregular grid point. So like linear problems, the difference scheme is determined by solving a small linear system for each irregular grid point. Wiegmann and Bube have proved in both the steady-state and time-dependent problems that when the mesh width is sufficiently small, these small linear systems can always be solved. This leads to a nonlinear system for the unknowns U_i , which can be solved very efficiently by the Levenberg-Marquardt algorithm with Armijo-Goldstein backtracking. Second order convergence is observed. Wiegmann and Bube have applied this framework to steady-state and time-dependent traffic flow problems; again second order convergence is observed.

10 Multi-dimensional methods for conservation laws and CLAW-PACK

LeVeque has continued his research on hyperbolic systems of conservation laws and the development and analysis of high resolution numerical methods for their solution, particularly the development of multi-dimensional wave-propagation methods that are based on one-dimensional ideas and yet give good multi-dimensional behavior[37], [38].

LeVeque has recently developed a software package, CLAWPACK, for solving systems of conservation laws in both one and two space dimensions using these methods[34], [39], [40]. A three-dimensional version has just been completed in work with Jan Olav Langseth at Oslo University[32],[33]. The routines require that the user provide subroutines to solve the Riemann problems and specify the boundary conditions. Numerous examples are included in the package, with sample Riemann solvers for standard systems of equations such as the Euler equations, the isothermal equations, and shallow water equations. Source terms can also be automatically included (using a Strang splitting), in which case the user also provides an ODE solver to be applied in each time step. Matlab m-files are also provided to display the results easily in both one and two dimensions.

This software is freely available through netlib, or on the Web at

<http://www.amath.washington.edu/~rjl/clawpack.html>

This package is intended for teaching purposes as well as research, and one goal has been to make the high-resolution shock capturing technology developed largely for gas dynamics and aerodynamics easily available to a much wider community. In the course of this work several extensions have been made to the standard flux-differencing form that is standardly used for conservation laws. In particular, an extension to hyperbolic systems that are not in conservation form has been developed that is useful, for example, in solving acoustics or elasticity problem in heterogeneous media. This is now being used in conjunction with IIM's for these problems.

The CLAWPACK package has also recently been integrated with Marsha Berger's adaptive mesh refinement code. The resulting code AMRCLAW will soon be freely available as well (in two space dimensions for the time being). The AMR code was originally developed for the Euler equations of gas dynamics and is described for example in [5], [6], [7], [12], [13]. The synthesis with CLAWPACK allows this adaptive refinement technology to be applied to a wide range of other hyperbolic problems, including for example groundwater flow and nonconservative problems such as the acoustics with discontinuous wave speeds. A paper is now in preparation[14] which describes this synthesis.

11 Acoustics

Acoustics in a two-dimensional heterogeneous medium is governed by the variable coefficient linear hyperbolic system of the form $q_t + A(x, y)q_x + B(x, y)q_y = 0$. We are particularly interested in the case where the material parameters (density and bulk modulus) are discontinuous across one or more interfaces. Solutions are not smooth at the interfaces, where waves split into reflected and transmitted pieces.

Surprisingly, CLAWPACK alone works quite well for such problems since it is based on resolution of data into multi-dimensional waves[40]. However, grid refinement studies show that only first order accuracy is achieved in the pressure, while the velocity, which is discontinuous at the interface, suffers some smearing as expected from a "capturing" method. With an IIM it is possible to obtain better accuracy, and such a method has been developed by LeVeque's student Chaoming Zhang[44]. CLAWPACK is used at points away from the interface, while a modified stencil is used at the interface. Figure 5 shows one example. Comparisons of the two approaches will be presented in [43].

12 Computation of seismic traveltimes in discontinuous media

Bube has applied the IIM strategy in computing seismic traveltimes in discontinuous media using finite difference approximations to the eikonal equation

$$(\tau_x)^2 + (\tau_z)^2 = s(x, z)^2,$$

where $\tau(x, z)$ is the first arrival traveltime to be determined and $s(x, z)$ is the given slowness field (the reciprocal of wave speed). This is a nonlinear hyperbolic equation. Bube [22] has extended a finite difference scheme developed by Vidale [68] for smooth media to be second order accurate when interfaces are present. As in the other applications of the IIM, a uniform Cartesian grid is used and special finite difference schemes are used near interfaces. The non-linearity of the jump conditions at the interface leads to complications in maintaining second order accuracy near the interface: the small systems to solve to determine the difference scheme at points near the interface are nonlinear. Fortunately these complications are surmountable by using an even larger stencil than might be expected from applications of the IIM to linear problems.

13 Convergence of numerical methods for inverse problems

In earlier work [20], Bube had shown second-order convergence of a method of inversion for Webster's horn equation based on a formally second order accurate numerical method for the forward problem. The forward problem has a discontinuity propagating along a characteristic of the same order as the initial discontinuity in the pressure source wavelet. In [19], Bube has continued some work started with a former graduate student, the late Dr. Robert Brookes. The purpose of this work is to determine how the order of discontinuity in the pressure source and the alignment of this discontinuity with the computational grid affect the order of convergence for the inverse problem. Second order convergence has been proved for pressure sources with discontinuities in the source or its first derivative. Only first order convergence is obtained when the discontinuity is in a higher derivative of the pressure source unless the medium is homogeneous near the surface, in which case convergence is second order. These issues are important for applications because the pressure sources which can actually be generated are smoother than a step function. This work was presented in an invited lecture in March 1995 at a workshop on inverse problems at IMA at the University of Minnesota.

In a three-dimensional stratified acoustic medium whose material properties depend only on depth, the surface response to a point source in pressure at the surface can be Radon transformed into plane wave responses. Each plane wave response is the solution of a one-dimensional wave equation. In [21], Bube has studied the effect of discontinuities in the medium on the order of convergence of numerical methods for recovering the density and wave speed for an acoustic medium from several plane wave responses. For smooth profiles, numerical methods can be constructed which are second order convergent. If the medium has discontinuities, the alignment of the discontinuities with the computational grid is crucial. Bube has developed a second order accurate method and proved second order convergence for a special case when the location of the discontinuities is known and satisfies some alignment constraints; when these constraints are violated, convergence reverts to first order.

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FIG. 2. Discontinuous solution to an elliptic equation computed on a uniform Cartesian grid using multigrid. Second order accuracy at all points is observed.

FIG. 3. Potential flow around a collection of solid bodies. Velocity vectors as computed on uniform grid.

FIG. 4. Left: A stretched elastic boundary is initially deformed to a star shape and relaxes to a circle in Stokes flow. The dotted circle is the unstretched interface. Incompressible fluid trapped within the stretched band determines the final size. Right: Accuracy study for a similar problem, starting with an elliptical interface. Log-log plot of the error in interface location at $t = 1$. Comparison is made to the Immersed Boundary Method (IBM) using discrete delta functions.

FIG. 5. Plane wave hitting an interface that is not aligned with the grid, as computed by CLAWPACK with modified stencils near the interface based on the IIM. The upward moving incident wave is split at the interface into a slower transmitted wave and a much weaker reflected wave. Note the pressure is continuous but the velocity is discontinuous at the interface. Results are on a 100×100 grid. Top: pressure contours and slice along $x = 0.35$. Bottom: velocity u contours and slice along $x = 0.6$. The solid lines are the exact solution in the slices.

FIG. 6. Computed streamlines and transport for saturated flow. A pressure drop is specified between the left and right boundaries with no flow at top and bottom. Embedded elliptical regions have permeabilities varying between 0.01 and 50 against background permeability 1. Streamlines are computed using IIM and multigrid for the streamfunction. Transport of tracer moving in from left boundary (injected for $0 < t < 3.0$) is computed using AMRCLAW package. Adaptive mesh refinement is partially visible. The regions near the front where no mesh is shown have refinement by an additional factor 2 over the adjacent regions, for an effective 160×160 grid.