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 Immersed Interface Methods
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Progress Report
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1. Overview. Considerable progress has been made on several problems mentioned in the original proposal and in last year's progress report. Our work is also going in some new directions. The primary focus is still on Immersed Interface Methods (IIM's) for high order accuracy of interface problems on Cartesian grids, but the investigators have also been involved in other projects. In particular, LeVeque's work on clawpack described below has been supported in part by these grants and has been used in direct connection with IIM's in projects in both groundwater flow and acoustics.

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2. Immersed interface methods.

2.1. Multigrid methods for Poisson problems. A full multigrid method (FMG) has been developed and implemented by Adams [1] for solving the discrete system of equations that arise from an IIM discretization of elliptic equations. The method can handle elliptic problems of the form

$$(1) \quad \begin{aligned} (\beta u_x)_x + (\beta u_y)_y &= f(x, y) \text{ in } \Omega \\ [u]_\Gamma &= w(s) \\ [\beta u_n]_\Gamma &= v(s) \end{aligned}$$

where Ω is a rectangular computational domain discretized by a Cartesian grid, and Γ is an internal immersed interface across which the solution u , the flux βu_n , or the source term f may have known jumps. Dirichlet or Dirichlet-Neumann boundary conditions can be specified on the boundary of Ω .

V-cycle rates of .06-.13 have been achieved due to the use of an interpolation operator that uses knowledge of the location of the interface as well as the jumps there. This operator reduces to ordinary bilinear interpolation for cells that contain no interface. For cells containing an interface, the value of u at a fine grid point, u_f , is calculated as a linear combination of the 4 cell corners, u_i , plus a correction term c ,

$$(2) \quad u_f = \sum_{i=1}^4 \gamma_i u_i - c$$

where the γ 's are determined by solving a 4×4 linear system of equations and c is determined as a function of the γ 's and the jumps at the interface. The interpolated value u_f is an $O(h^2)$ approximation to the solution u of the PDE in (1). We have used this method to solve model problems where the jump in β at the interface was as large as 2000 and the solution, the flux, and the source term had jumps at the interface as well. The method was also used to solve groundwater flow problems for the pressure where the permeability had jumps at the interface. (See Section 2.3 below.) These results were reported at the recent Copper Mountain Conference on Multigrid Methods in April 1995[1].

Recently, we have had lengthy discussions with Joel Dendy, Jr. at Los Alamos National Laboratory concerning multigrid methods for problems with discontinuities. The approach to interpolation used by Dendy and others is called "operator-induced" interpolation. The idea is to infer an interpolation scheme directly from the stencil used to discretize the PDE. In fact, Dendy's Black Box Multigrid code for non-symmetric problems could theoretically take our IIM stencil for the fine grid problem and produce a multigrid solution. It should be noted, however, that his code has mainly been used for problems where the discontinuities align with the grid which is not the case in our problems. We have obtained this code and in the near future plan to compare our approach with his.

At the moment, our coarse grid problems are gotten by applying the IIM method directly to the coarse grid. Shortly, we plan to enforce the Galerkin condition in generating the coarse grid problems to see if even coarser grids can be used. Getting the coarse grid problems in this way may also permit different smoothers to be used for more complicated problems. So far, point Gauss-Seidel smoothing has been sufficient.

This multigrid project has greatly benefitted from the weekly research seminars we have attended during our sabbatical at the University of Colorado, Boulder and the University of Colorado, Denver. In particular, we have benefitted from discussions with Steve McCormick, Tom Manteuffel, John Ruge, and Tom Russell.

2.2. Domain embedding. Adams and her Ph.D. student, Zhiyun Yang, are studying the use of IIM type ideas for elliptic problems that are posed on the inside or outside of a complicated domain. The idea is to immerse the domain in a square computational domain and use a Cartesian grid on the entire domain. In this sense, the approach is similar to Capacitance matrix methods, domain embedding techniques, and fictitious domain methods.

For these problems, it is common to know the boundary conditions on the immersed boundary (original problem domain), but not the jump conditions at the interface as required by the IIM method. The first step is to decide how to extend the problem to the entire domain. This step is crucial since it can greatly affect the condition number of the resulting system of equations. We introduce an auxiliary variable that is often one of the unknown jumps at the interface, and extend the problem by setting the other unknown jump to zero. The system of equations then has the form

$$(3) \quad \begin{pmatrix} A & -S \\ R_1 & R_2 \end{pmatrix} \begin{pmatrix} u \\ \phi \end{pmatrix} = \begin{pmatrix} f \\ g \end{pmatrix}$$

where the first equation is the discretization of the PDE in the entire domain with u the variable of interest. The second equation is an $O(h^2)$ discretization of the given boundary condition on the immersed boundary and ϕ is either $[u]_\Gamma$ or $[\beta u_n]_\Gamma$ depending on the nature of the boundary condition. Typically, for Dirichlet conditions, we extend so that $[\beta u_n]_\Gamma = 0$ and $[u]_\Gamma$ is the unknown auxiliary variable. For Neumann data, we do the reverse.

To solve (3), we first solve the Schur complement system,

$$(4) \quad (R_2 + R_1 A^{-1} S) \phi = g - R_1 A^{-1} f$$

for ϕ . Then the first equation can be used to retrieve u . The first equation can be solved by an FFT if A is the Laplacian operator. In general, the first equation can be solved by Adams' multigrid method [1] since the jumps at the interface are all known once ϕ is determined.

We have been successful in solving the Schur complement system (4) with a conjugate gradient procedure (using the normal equations since the matrix is nonsymmetric). This procedure does not require the Schur complement to be formed – it can remain in factored form. This is a big advantage, since the formation would require many solves with A^{-1} . Preliminary results are reported in [2]. We have used this procedure to get $O(h^2)$ solutions to flow problems over cylinders, and to solve interior Dirichlet problems on circular and elliptical domains. We have also applied the procedure to flows over multiple cylinders.

Presently, we are investigating a total multigrid solution process, where ϕ is also solved using multigrid. We have a preliminary code running. The main issue we are now resolving is the proper smoother to use with multigrid in this context.

2.3. Groundwater flow. Applications to groundwater flow are being investigated, starting with one-phase saturated flow governed by Darcy's law,

$$(5) \quad \vec{u} = \frac{\kappa}{\mu} \nabla p$$

where the permeability κ is discontinuous across some interface. The pressure p is determined by solving the elliptic equation $\nabla \cdot \left(\frac{\kappa}{\mu} \nabla p \right) = 0$, which results from incompressibility. This is solved using the IIM and the multigrid method developed by Adams. After p is computed at all points on the uniform grid, the velocity $\vec{u}$ can be computed at an arbitrary

point using (5) and an interpolation algorithm which takes into account the location of the interface and the jump conditions across the interface. This algorithm, developed by Adams, is analogous to the interpolation algorithm needed in multigrid as described above.

Once the velocity field has been computed, it can be used in an advection algorithm to model the transport of a contaminant with concentration q according to

$$(6) \quad q_t + \vec{u} \cdot \nabla q = 0.$$

This is currently done using the uniform grid multi-dimensional advection algorithm of [10], as implemented in `clawpack`. Some results are presented in [1].

Preliminary experiments indicate that even better results can be achieved in cases where there are large jumps in permeabilities by using a finite volume method in which some uniform cells are subdivided by the interface into two cells. These experiments were performed with the two-dimensional front-tracking code of LeVeque's former student Shyue[15], [22], and work is continuing in this direction.

LeVeque has also been working with Steve Yabusaki at PNL in Richland to use a more realistic velocity field with small-scale heterogeneities as a test problem for the advection algorithm in `clawpack`.

We have had regular discussions with Tom Russell and his students at CU-Denver on issues related to groundwater flow, both in regard to discontinuous coefficients in solving the elliptic flow equations, and in regard to advection algorithms for transport. Connections between Russell's ELLAM algorithms and "large time step" methods developed by LeVeque (e.g., [11]) are being explored. We have also discussed a problem in fractured media arising in modeling the Yucca Mountain Nuclear Repository where it may be possible to develop an immersed interface method.

2.4. Acoustics. LeVeque and his student Chaoming Zhang have been developing IIM's for acoustic wave equations with discontinuous wave speeds. The acoustic equations are written as a first order hyperbolic system and solved using `clawpack` over most of the grid. At grid points near the interface, special difference formulas are developed using the IIM approach based on jump conditions across the interface.

Second order accuracy has been achieved at all points on a uniform grid for several test problems, such as a plane wave striking an interface at an angle to the grid, and a radially-symmetric wave moving out of a circular region with different wave speed. Some of these results will be presented at the Computational Mechanics Conference of the American Society of Civil Engineers in May, 1995[17]. A detailed paper on this topic is nearly finished[16].

2.5. Elastic waves. Zhang is extending his work on acoustic waves to elastic waves, a more complicated system of equations that can be used in seismic modeling problems. Eventually these techniques will be applied to the inverse seismology problems studied by Bube. A preliminary version of the elastic wave code has been developed and recently tested on one simple problem. Further tests are underway.

2.6. Stokes flow. LeVeque and Zhilin Li have recently completed a paper[14] on Stokes flow using immersed interface methods. The model problem of a relaxing elastic membrane studied by Tu and Peskin has been solved using this approach with fully second order accuracy. Our approach can also be used to solve bubble problems where surface tension provides the singular force at the interface, rather than an elastic membrane. In this case there may also be discontinuities in the density and viscosity of the fluid across

the interface. These results will be presented at the Sixth International CFD Conference in Lake Tahoe this fall[21].

A quasi-Newton method was developed to efficiently implement an implicit algorithm that allows reasonable time steps. This algorithm should be useful in other versions of Peskin's Immersed Boundary Method as well.

The zero Reynolds number Stokes equations do not include inertial terms, i.e., the time derivatives of velocities in the momentum equations. We believe that we know how to incorporate these terms as well, which would be the next step towards solving the full incompressible Navier-Stokes equations with an immersed interface method. This is currently being studied.

2.7. Solidification. Zhilin Li's thesis[19] contained a preliminary look at one-dimensional solidification problems using the IIM. He has since extended this work[20] and applied it to a glaciology problem in work with Dave McTigue in the Geological Sciences Department at the University of Washington.

It should be possible to develop a two-dimensional version of this algorithm quite easily in conjunction with the algorithm for Stokes flow with inertial terms that was mentioned in Section 2.6. The mathematical structure is very similar. This will be pursued.

Donna Calhoun, a second year graduate student in Applied Mathematics, is also beginning to work with LeVeque on solidification problems. She would like to develop a code that combines fluid dynamics and solidification algorithms on Cartesian grids to study solidification (or melting) coupled with flow in the liquid phase. This is an ambitious project but many of the building blocks are under development already. Calhoun will be a summer intern in 1995 at the Lawrence Livermore National Laboratory, working in John Bell's group where Cartesian grid methods for incompressible flow have recently been developed. Although we ultimately hope to develop our own, this will be a very good learning experience and will hope to foster collaboration between our groups.

2.8. Computation of seismic traveltimes in discontinuous media. Bube has continued his work on 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). As in the other applications of the IIM, a uniform Cartesian grid is used and special finite difference schemes are used near interfaces. Bube [5] has extended a finite difference scheme developed by Vidale for smooth media to be second order accurate when interfaces are present. The nonlinearity of the jump conditions at the interface leads to complications in maintaining second order accuracy near the interface, but these complications are surmountable by using a larger stencil. Bube is also studying the application of the IIM to the system of conservation laws obtained by differentiating the eikonal equation, an approach developed by Van Trier and Symes for smooth media.

2.9. Differential equations with convection nonlinearities. Ph.D. student Andreas Wiegmann and Bube have been studying extending the IIM to nonlinear equations with convection nonlinearities of the form $u \cdot \nabla u$ which arise from the total derivative in equations of fluid dynamics. In an initial study [23], they have considered the steady-state Burger's equation with discontinuous viscosity

$$(\beta(x)u_x)_x + uu_x = f(x), \quad a \leq x \leq b,$$

$$u(a) = u_a, \quad u(b) = u_b.$$

The key ansatz which makes the IIM tractable for this nonlinear equation is to look for a difference scheme of the form

$$\gamma_{i1}u_{i-1} + \gamma_{i2}u_i + \gamma_{i3}u_{i+1} + u_i(\gamma_{i4}u_{i-1} + \gamma_{i5}u_i + \gamma_{i6}u_{i+1}) = f_i + C_i$$

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 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 a steady-state traffic flow problem; again second order convergence is observed. Wiegmann and Bube plan to apply these ideas to time-dependent and higher dimensional problems in the near future.

2.10. Inverse conductivity problems. In consultation with Bube, Ph.D. students Andreas Wiegmann and Carlos Tolmasky have started studying the application of the IIM to inverse conductivity problems where an object, e.g. a land mine, of different conductivity than the surrounding medium is to be located from electromagnetic measurements. They have been using the IIM in two dimensions in the computation of the forward problem. Initial studies have shown that the computed solutions do not depend monotonically on the location of the object as they should. This led to the discovery of situations for two-dimensional elliptic problems for which the IIM breaks down: the linear system to determine the coefficients of the difference scheme at an irregular grid point may be singular. They are currently studying conditions under which this breakdown occurs, and possible conditions to prevent this breakdown; one promising possibility is to choose the side of the interface on which to base the Taylor expansions by the sign of the jump in the conductivity. After understanding the IIM for the forward problem better, they plan to return to its application to the inverse problem.

3. Convergence of numerical methods for inverse problems. In earlier work, Bube has 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. Recently, Yeung and Bube [24] proved second order convergence for the forward problem with this propagating discontinuity and refined Bube's earlier results for the inverse problem when the pressure source wavelet is a step function. Crucial in these results are the alignment of the computational grid and the characteristic along which the discontinuity propagates. This propagating discontinuity complicates the study of numerical methods for both the forward and inverse problem, and offers an opportunity for the IIM to give accurate numerical solutions.

In [3], 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, but only first order convergence is obtained when the discontinuity is in a higher derivative

of the pressure source. 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 at the Workshop on Inverse Problems in Wave Propagation held in March 1995 at the Institute for Mathematics and its Applications 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. Recently, Chaderjian and Bube [6] showed that density, wave speed, and an attenuation coefficient can be recovered from several plane wave responses in a formal linearization of the continuum problem.

In [4], 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 without attenuation 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 satisfy some alignment constraints; when these constraints are violated, convergence reverts to first order. Bube is studying using the IIM to remove these constraints and still obtain second order convergence.

4. **CLAWPACK.** LeVeque has continued to develop multi-dimensional wave-propagation methods for hyperbolic systems of conservation laws. In particular, a software package `clawpack` (Conservation LAWs PACKage) has been released through `netlib`[8] and is still undergoing development with extensive modifications planned for the next release. This software was intended primarily as a tool for teaching and algorithm development, but it is apparently being used for a variety of uses already. An extension to handle logically-rectangular quadrilateral grids (instead of purely cartesian grids) which is currently under development should make it much more useful for solving real problems.

The current version includes both one-dimensional and two-dimensional codes, and also allow source terms in the hyperbolic system. A three-dimensional version has recently been completed by Jan-Olav Langseth at the University of Oslo, who will be visiting LeVeque in Boulder for two weeks this spring to complete its incorporation into `clawpack`. Three-dimensional results for the Euler equations will be presented at the Euler Equation Workshop at the University of Montreal in September, 1995[7].

LeVeque gave an invited lecture on `clawpack` at the Fifth International Conference on Hyperbolic Problems in Stony Brook in June of 1994[13].

LeVeque is now working with Piotr Smolarkiewicz at NCAR to incorporate the advection algorithm for `clawpack` into Smolarkiewicz's code for the anelastic equations modeling unstable flows over mountains. The "Stommel Gyre", a model for jet stream flow in oceanography, is also being used as a model problem as suggested by Matthew Hecht at NCAR.

A variety of other applications are being solved with `clawpack` and sample routines are being developed for inclusion in the package. A series of "User Notes"[9] is being developed that discuss various aspects of the algorithms. These will be expanded to cover each application as well. Eventually these notes will form the basis for an expansion of the text [12] to cover multi-dimensional problems and applications.

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