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13. ABSTRACT (Maximum 200 words)

A second order finite difference method has been developed for elliptic interface problems that involve discontinuous coefficients, singular source terms, non-smooth or even discontinuous coefficents across an arbitrary interface. The method is based on Cartesian grids and coupled with a multigrid solver. The new method will preserve the discrete maximum principle. The convergence of the new method has been proved.

Two different finite element spaces and corresponding Galerkin methods for elliptic interface problems using Cartesian grids have been developed. Some theoretical results about these finite element methods are also obtained. We believe that we are the first to develop these new finite element spaces over Cartesian grids.i

Some public subroutines of fast solvers for Helmholtz and Poisson equations on irregular domains either exterior or interior with various boundary conditions have been developed and made public.

In collaboration with J. K. Hunter of UC Davis and H. K. Zhao of UC Urvine, we formulate a model for the spreading on a surface of a drop that deposits an autophobic monolayer of surfactant. We present numerical solutions of the model equations using an immersed interface method and a level set method.

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Final Report of ARO Grant 39676-MA: Finite Element Methods and Iterative Refinement Techniques for Partial Differential Equations Involving Interfaces

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1 Statement of the problem studied and Significance

This project concerns development and application of finite difference methods using Cartesian grids for differential equations with complicated geometry or/and with interfaces.

A model problem is the Poisson equation

$$\nabla \cdot (\beta \nabla u) = f(x, y), \tag{1}$$

with the following two important settings:

- The solution domain is arbitrary with Neumann or mixed boundary conditions, see Fig 1 (a). It is well known that the finite difference methods generally will lose accuracy for arbitrary boundaries.
- Interface problems defined on a rectangular domain, see Fig 1 (b). The coefficient $\beta(x, y)$ may be discontinuous across the interface. Whenever we have situations involving two different materials, or the same material but in different states, the physical properties will be different across the interface, we have to deal with interface problems. For example, the interface between oil and water, the interface between a fluid and a gas bubble are examples of different materials. The ice-melting, crystal growth, and other solidification problems are examples of interface problems of the same materials but at different states.

The problems we are interested in come from different applications and they have one, several, or all of the following properties:

- There is one or more complicated geometries, boundaries or interfaces.

- The coefficients of the differential equations may be discontinuous across interfaces.

- The solution and its derivatives may be discontinuous across interfaces.

- There may be discontinuous or singular sources, or dipoles along interfaces, for example

$$f = f_c + \int_{\Gamma} \delta(\mathbf{x} - \mathbf{X}) d\mathbf{X},$$

  where Γ is a curve in two dimensions, and a surface in three dimensions, δ is the Dirac-delta function which is not a standard mathematical function and is only defined in terms of the distribution theory.

- The interfaces may be fixed or moving and may develop topological changes such as merging or breaking.

1.1 Why Cartesian grids?

It is true that the finite element method may be used to solve the problems of the interest. However we want to develop finite difference methods for the following reasons:

- There is almost no cost in the grid generation. This is very significant for moving boundary/interface problems.

- To get sharp interfaces and solutions, we want to use the infinity norm instead of energy norm used in the finite element method. A method converges with high order accuracy in the energy norm may not converge at all in the infinity norm.

- We want to take advantage of many efficient packages/solvers which are written for Cartesian grids.

- Recently, *the level set method* has been very successful for a number of moving interface/boundary problems, especially for the problems with topological changes and three dimensional problems. The level set function works best with Cartesian grids.

- Finite difference schemes are generally easier to learn and implement than the finite element method.

2 Summary of the most important results

2.1 Algorithms development

2.1.1 Immersed finite element methods for interface problems

We have developed *two different finite element spaces* for interface problems and developed the corresponding Galerkin finite element methods for elliptic interface problems using Cartesian grids. Some theoretical results about these finite element methods are also obtained. We believe that we are the first to develop these new finite element spaces over Cartesian grids. With the new finite element spaces, we are able to derive stable and accurate numerical methods with sharp interfaces, see [12, 4]. In the non-conforming finite element space, a basis function is defined almost exact the same as the standard piecewise linear finite element space except that we enforce the natural jump conditions across the interface. This finite element space have the following properties:

- It has the same support as the standard piecewise linear finite element space. Therefore it is very easy to programming.
- A global basis function may not be continuous across the edges whether the interface cuts through. Therefore it is a non-conforming finite element space.
- Existence and uniqueness of the basis function has been established.
- Theoretically, for a solution of an elliptic interface problem, we can construct an interpolation function that approximates the solution to second order, and the first derivatives of the solution to first order within each triangle.
- The method is second order in the L^2 norm and the energy norm. In terms of the L^∞ norm, a linear to super-linear convergence is expected.
- The finite element method can be directly applied to three dimensional problems.

In the conforming finite element space for interface problems, we have shown that it is impossible to construct a conforming finite element space using polynomials which satisfies the natural jump conditions while it has the same support as the standard piecewise linear basis function using piecewise polynomials. As a breakthrough, we came to an idea to extend the support of the basis function to one more triangle along the direction of the interface. In this way, a piecewise linear and conforming finite element space can be constructed for interface problems. We think this is a major advance in this area. The conforming finite element space has the following properties:

- Existence and uniqueness of the basis function has been established.
- The finite element space is a conforming finite element space. Therefore most of the standard theories for conforming finite element spaces apply directly. High order elements can be constructed accordingly.
- Theoretically, for a solution of an elliptic interface problem, we can construct an interpolation function in the finite element space that approximates the solution to second order, and the first derivatives of the solution to first order within each triangle
- The method is second order in the L^2 norm and in the energy norm. Numerical examples show that it is also second order accurate in the the L^∞ norm.

2.1.2 Maximum preserving scheme for elliptic interface problems and applications

Some new difference methods have been developed for elliptic interface problems that involve discontinuous coefficients, singular source terms, non-smooth or even discontinuous coefficients across an arbitrary interfaces. The new methods are based on Cartesian grids and satisfy the sign property that guarantees the discrete maximum principle using an optimization approach. The resulting linear system of equations obtained from the new methods is diagonally dominant and its symmetric part is negative definite. The convergence of the new methods have been proved by constructing the comparison functions.

With this work, we have a unique second order finite difference method using Cartesian grids for elliptic interface problems that allows variable discontinuous coefficients. This work has solved the stability problem for the original immersed interface method and provided theoretical foundation for the immersed interface method. We believe the new method is the first second order method (in the maximum norm) using Cartesian grids for variable discontinuous coefficients that can guarantee the discrete maximum principal and second order convergence, see [11].

The method has been coupled with a multigrid solver. We have written a general subroutine for this methods with the interface been represented by a set of control points.

The generalization of the method to three dimensional problems is described in [2, 3].

The generalization of the method to diffusion and advection equations with a new multigrid solver is described in [1].

2.1.3 New Formulations and algorithm for interface problems in polar coordinates

The new methods are based on a formulation that transforms the interface problem with a non-smooth or discontinuous solution to a problem with a smooth solution. The new formulation leads to a simple second order finite difference scheme for the partial differential equation and a new interpolation scheme for the normal derivative of the solution. In conjunction with the fast immersed interface method, a fast solver has been developed for the interface problems with piecewise constant but discontinuous coefficient using the new formulation in polar coordinate system. The work is described in [14].

2.2 Applications of new algorithms

2.2.1 Level-set function approach to an inverse interface problem in shape identification

A model problem in electrical impedance tomography for the identification of unknown shapes from data in a narrow strip along the boundary of the domain is investigated. The representation of the shape of the boundary and its evolution during an iterative reconstruction process is achieved by the level set method. The shape derivatives of this problem involve the normal derivative of the potential along the unknown boundary. Hence an accurate resolution of its derivatives along the unknown interface is essential. It is obtained by the immersed interface method. The work for 2D and 3D problems are explained in [6] and [3] respectively.

2.2.2 Autophobic spreading of drops

In collaboration with J. K. Hunter of UC Davis and H. K. Zhao of Stanford University, we formulate a model for the spreading on a surface of a drop that deposits an autophobic monolayer of surfactant. We present numerical solutions of the model equations using an immersed interface method and a level set method, see [5].

2.2.3 Immersed Interface Method for Navier-Stokes equations with moving interface.

We have derived the jump conditions for Navier-Stokes equations with an interface in 2D and 3D, see [9]. The immersed interface method for the incompressible Navier-Stokes equations with singular forces along one or several interfaces in the solution domain has been developed in [8]. The new method is based on a second-order projection method with modifications only at grid points near or on the interface. From the derivation of the new method, we expect fully second-order accuracy for the velocity and nearly second-order accuracy for the pressure in the maximum norm including those grid points near or on the interface. This has been confirmed in our numerical experiments. Furthermore, the computed solutions are sharp across the interface.

Using the fast immersed interface method and the vorticity stream-function formulation, we have developed a fast method for Navier-Stokes equations defined on general domains in [13].

2.3 Software development

We have written some public subroutines of fast solvers for Helmholtz and Poisson equations on irregular domains either exterior or interior with various boundary conditions have been developed and made public through anonymous ftp.

These subroutines use the fast immersed interface method by introducing a unknown jump either in the solution or the normal derivative. Using the fast solver from Fishpack, we implicitly solve a linear system of equations using GMRES iteration. These methods are called fast solvers because of the number of iterations is independent of mesh size. While there are similar methods for problems with Dirichlet boundary conditions, our approach for problems with Neumann boundary conditions using some preconditioning techniques is not only unique, but also necessary to guarantee the number of iterations to be independent of mesh size. These packages include

- Fast solves for Helmholtz/Poisson equations defined in an arbitrary interior domain with Dirichlet boundary condition.

- Fast solves for Helmholtz/Poisson equations defined in an arbitrary exterior domain with Dirichlet boundary condition.

- Fast solves for Poisson equations defined in an arbitrary exterior domain with Dirichlet/Neumann boundary condition.

Our method also works for Helmholtz equations defined in an arbitrary exterior domain, but the number of iteration depends on mesh size. Whether we can derive a fast solver for this type of problems is an open question.

Other applications and contributions can be found in [10, 15, 16, 7] etc..

3 Participating scientific personals

Zhilin Li (PI, NCSU); Kazufumi Ito (Co-PI, NCSU), Tao Lin (collaborator, VPI); Shaozhong Deng (Ph.D, graduated in 2001 from NCSU, now a postdoc at UNC-Charlotte), Xingzhou Yang, Yaw Kyei, Guo Chen, Yan Gong (Ph.D graduate students at NCSU, three of them will graduate in the summer, 2003).

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