Inverse Scattering in Near-field Optics

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Abstract

A regularized continuation method is developed for a two-dimensional inverse medium scattering problem in near-field optics, which reconstructs the scatterer of an inhomogeneous medium deposited on a homogeneous substrate from data accessible through photon scanning tunneling microscopy (PSTM) experiments. In addition to the ill-posedness of inverse scattering problems, two difficulties arise because of the layered background medium and limited aperture data. Numerical experiments are included to illustrate the robust behavior of the method. Related topics will also be discussed. This is a joint work with Peijun Li of University of Michigan.

Equivalence of Half-Quadratic Minimization and the Relaxed Fixed Point Iteration

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Abstract

In this talk, we focus on the minimization of regularized objective functions using the popular half-quadratic approach introduced by Geman and Reynolds in 1992. We show that whenever applicable, this approach is equivalent to the very classical gradient linearization approach, known also as the fixed point iteration.

Are New Energy Sources Within Reach?

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Abstract

The world needs enormous new crude oil reserves. During the next several decades, there is not and there will not be an economical, abundant substitute for crude oil in the economies of industrial countries, even with the price of a barrel of oil over US$60. Maintaining the supply needed to support these economies and enable them to grow means that significant additional crude reserves must be developed. The conventional (light and medium) oil resources discovered up to the end of 2002 will last at most 40 years at 2002's production rate. Thus additional development will be primarily in the form of the sole alternative: heavy crudes.

While the vast heavy and ultraheavy oil fields will dominate the world's oil production in the next several decades, many of the heaviest hydrocarbons are waiting for new technologies that will transform them into economically feasible projects. A mathematically and numerically based understanding of the production

mechanisms for these reserves is urgently required. In this talk the speaker will present an overview on the current problems and the state-of-the-art techniques on the development of laboratory experiments, mathematical modeling, and numerical methods, and computer simulations for heavy oil reservoirs.

An Adaptive Perfectly Matched Layer Technique for 3-D Time-Harmonic Electromagnetic Scattering Problems

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Abstract

We develop an adaptive perfectly matched layer (PML) technique for solving the time harmonic electromagnetic scattering problems. The PML parameters such as the thickness of the layer and the fictitious medium property are determined through sharp a posteriori error estimates. Combined with the adaptive finite element method, the adaptive PML technique provides a complete numerical strategy to solve the scattering problem in the framework of FEM which produces automatically coarse mesh size away from the fixed domain and thus makes the total computational costs insensitive to the thickness of the PML absorbing layer. Numerical experiments are included to illustrate the competitive behavior of the proposed adaptive method. This is a joint work with Chen Junqing.

Numerical Approximations of a Phase Field Bending Elasticity Model of Vesicle Membranes

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Abstract

In this talk, we discuss recent works on the numerical approximations of a phase field bending elasticity model of vesicle membranes. We focus on the use of mixed finite element methods and present some convergence analysis. Recent results on adaptive FEM based on a posterior error estimates are also presented. The effectiveness of the numerical simulations is illustrated via examples related to the biological and mechanical studies of vesicle membranes. References can be found in http://www.math.psu.edu/qdu/Res/Pic/gallery5.html.

Some Thoughts about the Curriculum in Computational Mathematics

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Abstract

In recent years, I have been working with some friends on building a better undergraduate and graduate curriculum in computational and applied mathematics, both at Princeton University and Peking University. I will discuss what we have learned during this process, and what more needs to be done.

Dynamic Generation and Depletion of Small Scales for 3D Incompressible Flows

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Abstract

Whether the 3D incompressible Euler equation can develop a finite time singularity from smooth initial data has been an outstanding open problem. Here we review some existing computational and theoretical work on possible finite blow-up of the 3D Euler equation. We show that there is a sharp relationship between the geometric properties of the vortex filament and the maximum vortex stretching. By exploring this local geometric property of the vorticity field, we have obtained a global existence of the 3D incompressible Euler equations under some localized conditions on the velocity and the unit vorticity vector field. Further, we perform large scale computations of the 3D Euler equations to re-examine the alleged finite-time blowup of the two antiparallel vortex tubes, which has been considered as one of the most attractive candidates for a finite-time

blowup of the 3D Euler equations. Our numerical studies indicate that the maximum vorticity does not grow faster than double exponential in time. The local geometric regularity of vortex lines seems to be responsible for the dynamic depletion of vortex stretching. Finally, we will present a new class of solutions for the 3D Euler and Navier-Stokes equations, which exhibit very interesting dynamic growth property but have global existence for all times.

Superconvergence and Adaptivity

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Abstract

In this talk we shall provide an adaptive finite element method based on the superconvergence on the very general meshes. These meshes can be generated by most popular mesh generators. Our numerical tests show the efficiency of the algorithms. Especially we observed some superconvergence phenomena at nodes for linear elements solutions which is suprising since the function aprroxiamation is known to be no superconvergence for linear elements from the point of view of nagative norm error estimates.

A Semiclassical Transport Model for Thin Quantum Barrier

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Abstract

We present a time-dependent semiclassical transport model for mixed state scattering with thin quantum barriers. The idea is to use a multiscale approach to connect regions for which a classical description of the system dynamics is valid across regions for which the classical description fails, such as when the gradient of the potential is undefined. We do this by first solving a stationary Schrodinger equation in the quantum region to obtain the scattering coefficients. These coefficients allow us to build the interface condition to the particle flux, as done in the Hamiltonian-preserving schemes of Jin and Wen for classical barriers, that bridges the quantum region, connecting two classical regions. Away from the barrier, the problem may be solved by traditional numerical methods. The overall numerical cost is roughly the same as solving a classical barrier.

A Coupling System of Elliptic Boundary Value Problem and Navier-Stokes Equations for the Geometry Design of Blades Surface

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Abstract

We present a time-dependent semiclassical transport model for mixed state scattering with thin quantum barriers. The idea is to use a multiscale approach to connect regions for which a classical description of the system dynamics is valid across regions for which the classical description fails, such as when the gradient of the potential is undefined. We do this by first solving a stationary Schrodinger equation in the quantum region to obtain the scattering coefficients. These coefficients allow us to build the interface condition to the particle flux, as done in the Hamiltonian-preserving schemes of Jin and Wen for classical barriers, that bridges the quantum region, connecting two classical regions. Away from the barrier, the problem may be solved by traditional numerical methods. The overall numerical cost is roughly the same as solving a classical barrier.

Superconvergence in FE Approximation of Optimal Control

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Abstract

In this talk, we review some superconvergence results in finite element approximation of contrained optimal control. There seem two classes of superconvergence convergence results in FE approximation of optimal control. One is associated with the standard FE superconvergence and thus has the usual restrictions meshes used. The other is quite unique in optimal control and has no restrictions on meshes at all.

Extrapolations for Solving the Weakly Singular Volterra Integral Equations

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Abstract

Based on a new generalization of discrete Gronwall inequality and Navet's quadrature rule of computing integrals with the end point singularity , a new quadrature method for solving nonlinear weakly singular Volterra integral equations of the second kind is presented . The convergence of the approximation solution and the asymptotic expansion of the error are proved, so by means of the extrapolation technique we not only obtain a higher accuracy order of the approximation but also a posteriori estimate of the error are got.

High Order Accurate Anti-diffusive WENO Methods and Application to Shallow Water with Transport of Pollutant

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Abstract

In this talk, we first describe a recently developed technique to sharpen contact discontinuities for high order finite difference WENO schemes solving multi-dimensional hyperbolic conservation laws and Hamilton-Jacobi equations. The objective is to obtain sharp resolution for contact discontinuities, close to the quality of discrete traveling waves which do not smear progressively for longer time, while maintaining high order accuracy in smooth regions and non-oscillatory property for discontinuities. We then describe an application of this technique to the simulation of shallow water equations with the transport of pollutant. This is a joint work with Zhengfu Xu of Penn State University.

On Finite Element Methods over 2-D Hexagon and 3-D Dodecahedron Partitions

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Abstract

FEM can deal with meshes consisting of arbitrary triangles or quadrilaterals elements in 2-D case and tetrahedra or hexahedra in 3-D. While as is well-known, some special 2-D hexagons and 3-D dodecahedrons partitions extensively exist in the nature as well as in many application fields, such as in material science and crystal structure. As an example, a rational hexagonal element has been proposed in nuclear engineering.

In this talk, we investigate how to construct finite elements over three direction mesh (hexagon partition) in 2-D and four direction mesh (dodecahedron partition) in 3-D. Based on our former work [?], by using the so-called three-directional coordinates in 2-D and four-directional coordinates in 3-D, we propose several conforming elements, such as a bi-linear B-spline element in 2-D and incomplete tri-linear B-spline element in 3-D. Both elements belong to C^0 and have so-called

super-continuous property of C^1 around some inner vertex. We also will present some special nonconforming elements. An edge-oriented hexagonal element in terms of bivariate quadratic in 2-D and a face-oriented dodecahedron element in terms of incomplete tri-variate cubic in 3-D are studied. In 2-D case the convergence analysis is similar to the rotated Q_1 quadrilateral element. To match our analysis some numerical examples will be given.

This is a joint work with my PhD student Yang Chao.

A Survey on Domain Decomposition and Multigrid Methods for Nonlinear Problems and Variational Inequalities

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Abstract

Domain decomposition (DD) and multigrid (MG) have been intensively studied for linear elliptic problems. In this talk, we will present a general framework, c.f. [3,4], to extend DD and MG methods to general nonlinear problems using the ideas of space decomposition and subspace correction [5].

For variational inequalities like the obstacle problems, there are some algorithms that can be used for solving it. However, a regirous convergence proof is still missing in the literature. In this work, we use the framework of space decomposition and subspace correction to give some general proofs of convergence for variational inequalities [1,2]. We use this theory to develope several domain decomposition and multigrid algorithms for obstacle problems. These algorithms have a convergence rate independent of the mesh parameters used in finite

element approximations. The convergence property is verified theoretically and numerically.

One of the essential difficulties in the convergence analysis for obstacle problems is the estimate for the constant appeared in the so-called partition lemma. For obstacle problems, we need to decompose a given function into a sum of functions from the subspaces. The decompositions should satisfy a norm equivalent estimate. In addition, the decomposed functions also need to satisfy some sub-obstacle constraints. By using a new nonlinear constrained interpolation operator, we are able to show that the constant from the partition lemma is independent of the mesh parameters of finite element approximations, see [1] for the details.

References:

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Moving Mesh Methods for Singular Problems Using Perturbed Harmonic Mappings

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Abstract

In this talk, we will extend Dvinsky's method to provide an efficient and practical moving mesh algorithm for solving partial differential equations.

The key idea is to construct the harmonic map between the physical space and a parameter space by an iteration procedure. Each iteration step is to move the mesh closer to the harmonic map. This procedure is simple, easy to program, and also enables us to keep the map harmonic even after long time of numerical integration.

We will also discuss a recent work in developing moving mesh strategies for solving problems defined on a sphere. To construct mappings between the physical domain and the logical domain, it has been demonstrated that harmonic mapping approaches are useful for a general class of solution domains. However, it is known that the curvature of the sphere is positive, which makes the

harmonic mapping on a sphere not unique. To fix the uniqueness issue, we follow Sacks and Uhlenbeck [Ann. Math., 113, 1-24 (1981)] to use a perturbed harmonic mapping in mesh generation. A detailed moving mesh strategy including mesh redistribution and solution updating on a sphere will be presented.

This work is joint with Y. Di, R. Li and P.-W. Zhang of Peking University.

An Economical Approach to Implement the 4-dimensional Variational Data Assimilation

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Abstract

Numerical weather prediction (NWP) is one of the most important tools to predict future states of atmosphere. It is produced by a numerical model starting from an initial condition (IC) that describes the current state of atmosphere. Prior to the prediction, however, the IC must be provided, which directly influences the accuracy of NWP. 4-dimensional variational data assimilation4-14 (4DVar) is one of the most efficient methods to provide optimal IC for NWP, but its huge computing cost for the nonlinear optimal iteration based on the adjoint technique greatly limits its wide applications. Here we propose an economical approach to implement the 4DVar, using the empirical orthogonal function (EOF). The proposed approach does not need to make the nonlinear optimal iteration to get 4DVar solution, which avoids calculating the gradient of the 4DVar cost function at each step of the iteration using

the adjoint technique. The easy and fast characteristics of the approach make it possible to widely use the 4DVar in operational NWPs in the world, which are preliminarily testified in some ideal tests. We anticipate the proposed approach to lead wider applications of 4DVar to many related fields. For example, the efficiency of the 4DVar with the proposed approach in ocean data assimilation could be tested. Furthermore, predictions or simulations based on initial value problems in other fields in science, engineering and economics might be also improved if the 4DVar is used for their initializations.

Superconvergence for a Stabilized Finite Element Method for the Stokes Equation by Using Coarsening Projections

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Abstract

It has been proved that superconvergence can be obtained for Galerkin finite element approximations by using L^2 projection methods over a certain "coarse" spaces. This process is essentially based on the well-known error estimates in negative norms: a high order of approximation accuracy in negative norms implies the existence of superconvergent points, curves, even sub-regions. The power of the L^2 projection method is to make a dynamic use of the existing superconvergent points/curves/sub-regions without knowing their exact location. The main objective of this talk is to outline this basic superconvergent technique and then demonstrate the difficulty when applied to problems for which no negative norm error estimates are known. In particular, a stabilized finite element scheme for the Stokes

equation shall be studied and a remedy strategy shall be designed and analyzed.

New Multigrid Methods and Theories for H(curl) and H(div) Systems

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Abstract

In this talk, a unified theory will first be given for geometric multigrid methods for H(grad), H(curl) and H(div) systems. Then a new preconditioner will be given for H(curl) and H(div) systems in terms of preconditioner for H(grad) system. As a result, the edge element systems for the Maxwell equation and the indefinite mixed finite element systems (for, say, the Darcy's law) can be solved efficiently in terms of preconditioners (such as algebraic multigrid methods) for the well-studied Poisson (like) equations. Both theory and numerical results will also be given to demonstrate the extraordinary efficiency and practicality of this new approach. This talk is based on a joint work with Ralf Hiptmair.

Adaptive Finite Element Method for P-Laplacian Equation

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Abstract

In this talk, we discuss the adaptive finite element method for p-Laplacian equations. It is well known that p-Laplacian equation is degenerated nonlinear partial differential equation, and it is difficult to obtain the reliable and efficient a posteriori error estimate by standard technique. Based on the quasi-norm technique, we provided the residual type and the recovery type a posteriori error estimates. The theoretical analysis and the numerical results demonstrate that the a posteriori error estimates based on the quasi-norm are reliable and efficient. Moreover, based on the superconvergence analysis, it is shown that the recovery type a posteriori error estimate is asymptotically exact under the strong conditions.

Domain Decomposition with Nonmatching Grids for Exterior Transmission Problems via FEM and DtN Mapping

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Abstract

In this talk, we are concerned with a non-overlapping domain decomposition method (DDM) for exterior transmission problems in the plane. Based on the natural boundary integral operator, we combine the DDM with a Dirichlet-to-Neumann (DtN) mapping and provide the numerical analysis with nonmatching grids. The weak continuity of the approximation solutions on the interface is imposed by a dual basis multiplier. We show that this multiplier space can generate optimal error estimate and obtain the corresponding rate of convergence. Finally, several numerical examples confirm the theoretical results.

Mathematical Theory of Non-Equilibrium Green Function in MOSFET

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Abstract

This talk is mainly about mathematical theory of non-equilibrium Green function(NEGF) which is popularly used in MOSFET(Metal-Oxide-Semiconductor Field Effect Transistor) simulation. To do MOSFET simulation, the coupled Poisson equation and Schrödinger equation have to be calculated self-consistently. For open systems, it is necessary to confirm the boundary condition for Schrödinger equation. Traditional zero boundary condition and period boundary condition can not describe non-equilibrium state. NEGF method provides a sound conceptual formalism for non-equilibrium state. The effect of contacts on conductor is considered by introduced self-energy. Spectral function, density matrix and current can be expressed by Green function in a simple form independent of dimension. Firstly, we gave the different boundary conditions of Green function for both 1-D and 2-D open systems, also proved the

equivalence of these boundary conditions. In fact, self-energy is the artificial boundary condition when Green function is confined to a finite domain. By analyzing the boundary condition of open systems Schrödinger equation, we arrived the conclusion that self-energy came from the artificial boundary condition of Schrödinger equation from open systems to finite systems. In succession, the density matrix is represented by Green function and wave function respectively. We proved that Green function method is equal to solve Schrödinger equation directly in case of ballistic transport. The wave function expression is more complicated than that of Green function and is difficult to extend to high dimension cases. The wave function expression has to consider the dispersion relation of each character. Green function has the merit on the simple computation formalism, while Green function has to cost large computation. The equivalence of Green function and wave function hints us to give an improved method to compute the density matrix avoiding to compute the total Green function. The improved method and NEGF formalism is applied to simulate the double gate MOSFET in our work.