Plenary Talks

A Personal and Historical View of Computational Mathematics

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Abstract. Computational mathematics is as old as mathematics itself but "modern" computational mathematics probably started after the Second World War, with the advent of modern computers. My own personal and professional life has coincided with this period. I have been fortunate enough to have participated in different aspects of the field and have witnessed fundamental changes and dramatic new directions, with impact both within and beyond the field itself. In this talk, I'd like to offer a personal and historical view of these developments, with an eye towards the future.

A Survey on The Spectral Theory of Nonnegative Tensors

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Abstract. This is a survey on the recent development of the spectral theory of nonnegative tensors and its applications. The H eigenvalue and the Z eigenvalue problems for tensors are studied separately. To the H eigenvalue problem for nonnegative tensors, the whole Perron-Frobenius theory for nonnegative matrices is completely extended, while to the Z eigenvalue problem there are many distinctions, and are studied carefully in details. Numerical methods are also discussed. Three kinds of applications are studied: higher order Markov chains, spectral theory of hypergraphs and the quantum entanglement.

Learning About Online Learning

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Abstract. We have been teaching a Massive Open Online Course (MOOC) in the past year with over 100,000 students globally enrolled. A few million students are in over a hundred MOOCs. We crawl and analyze data associated with discussion forums on these MOOCs, and study how we can provide more effective learning at massive scale.

Numerical Simulation of Flows in Highly Heterogeneous Porous Media

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Abstract. We shall present an overview of some approximation strategies and robust solution methods for the resulting algebraic system for numerical solution of flows in highly heterogeneous porous media. Our main goal is derivation of numerical methods that work well for both, Darcy and Brinkman equations, and could be used either as (1) a stand alone numerical upscaling procedure or (2) robust (with respect to the high contrast of the porous media) iterative solvers for the finite element approximation on a fine-mesh spatial scale. The preconditioners are based on overlapping domain decomposition technique. The robustness with respect to the contrast is achieved via special construction of a coarse grid space that includes patched together eigenfunctions corresponding to the smallest eigenvalues of properly weighted local spectral problems. This approach has a natural abstract framework which we shall discuss as well.

The main target of our applications are numerical upscaling and simulation of fluid flows in highly heterogeneous media modeled by Brinkman, Darcy, and steady-state Richards' equation (governed for example by Haverkamp and van Genuchten relations for the relative permeability).

A New Model for Coalescent with Recombination

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Abstract. In this talk I shall briefly report some of our recent research progress in biostatistics and computational biology. In particular I shall report our recent joint work in collaboration with CAS-MPG Patner Institute for Computational Biology and Beijing Jiaotong University. In this joint work we proposed a new model for describing coalescent with recombination. Based on this model we developed a new algorithm to generate ancestral recombination graphs. Our model employs heavily the theory of Markov jump processes. By showing the back in time model and spatial moving model share the same statistical properties, we provide a unified interpretation for the algorithms of simulating coalescent with recombination.

Computing Integrals in Many Dimensions – What's New?

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Abstract. In recent years methods of high-dimensional numerical integration have been developed to the point where integrals arising in some applications can be tackled even when the number of dimensions is in the hundreds or thousands (or even in principle infinite), and with a guaranteed rate of convergence close to $1/N$, where N is the number of integration points. The rules are equal-weight (or Quasi-Monte Carlo) rules, with associated algorithms for generating the points. A guiding example has been the flow of a liquid through a porous medium, modelled by a partial differential equation with a random permeability field.

Stream 1
Applications of Engineering Mathematics

Invited Talks

Modelling and Analysis of Heterogeneous Network: A Stochastic Geometric Approach

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Abstract. Current cellular systems are becoming decentralized and heterogeneous with the introduction of low-powered base stations like picocells and femtocells. The random node locations in these networks coupled with their decentralized nature make the analysis of interference and network performance challenging.

Spatial Poisson point processes is becoming a popular model for BS locations in these heterogeneous networks. In this talk, a model for heterogeneous networks based on multi-tier Poisson point process will be introduced. Using this model, the performance of multi-antenna heterogeneous network is analyzed with a MMSE receiver. This talk will also introduce new tools from stochastic geometry that facilitate the analysis of cellular networks.

Network Analysis and Visualisation

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Abstract. Recent technological advances have led to massive complex network models in many domains, including social networks, biological networks and webgraphs. Understanding these networks is a key enabler for many applications.

Good network analysis methods are needed for these networks to reveal the hidden structure of the networks, thus leading to new findings and possible predictions for the future.

On the other hand, such analysis methods can be effectively communicated to humans using network visualisation methods by amplifying human understanding.

A critical issue for both network analysis and visualisation methods of massive complex network is scalability and complexity. Existing methods do not scale well enough to be effective on current big data sets.

This talk will review fundamental concepts, methods and algorithms for network analysis and visualisation methods, and address the challenging issues for massive complex networks.

Linear Systems Model for Quantum Memories

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Abstract. Quantum memories are expected to be key components in quantum repeaters for use in large scale quantum networks. Experimental work is well advanced and delivering very promising results. This talk will describe a fully quantum mechanical model for quantum memories based on an infinite dimensional linear quantum stochastic system. Analytical results are provided to describe the fundamental write and read stages. These include explicit representations for impulse responses and transfer functions.

Game-Theoretic Understanding of Resource Pricing in Cellular Radios

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Abstract. The spectrum shortage in wireless communications is a fundamental assumption, and much of research has been focusing on spectral efficiency (bits/hertz). When it comes to users, however, the spectral efficiency is not the primary concern. The users definitely care more about economical benefit (bits/payment). Imagine an ample wireless pipeline is available, but it costs more than user's expectation. Then, the wireless service may not spread over the entire market. This talk is to highlight some of our recent results on wireless economics, with some emphasis on price competition & resource sharing, spectrum auction/leasing and user behavior.

Iterative SVD Algorithm for Optimal Control Synthesis of Bilinear Ensemble Systems

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Abstract. Designing optimal controls for manipulating an ensemble of bilinear systems is imperative for wide-ranging applications in quantum control and robotics. We develop an iterative optimization-free algorithm for synthesizing optimal ensemble controls of bilinear systems based on the singular value decomposition (SVD). At each step, the bilinear ensemble system is represented as a time-varying linear ensemble system, and the optimal controls for the bilinear ensemble system are obtained through iteratively solving the corresponding linear ensemble system using an SVD-based computational algorithm. The convergence of the algorithm is illustrated theoretically and through examples of pulse design in quantum control.

On Some Recent Constructions of Quantum Error-Correcting Codes

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Abstract. Quantum error-correcting codes were introduced to protect quantum information from decoherence and quantum noise. Ever since their introduction in the mid 1990s, much progress has been made on their construction. A rather prevalent idea that has proved to be very useful is to construct quantum codes using classical error-correcting block codes.

It has also been established from experiments that, in many quantum systems, phase-flip errors happen more frequently than bit-ip errors. Asymmetric quantum error-correcting codes, which take advantage of this asymmetry, have been introduced as a result (as opposed to the symmetric ones which do not distinguish between these two types of errors). Both symmetric and asymmetric quantum codes have been much investigated in recent years.

As in the case of classical error-correcting block codes, there are known bounds constraining the parameters of (both symmetric and asymmetric) quantum codes. The primary question we are interested in is the construction of optimal quantum codes, in the sense that codes of better parameters can be proved not to exist. Of course, a code that attains some known bound on the parameters is therefore optimal.

In this talk, we will discuss some recent constructions of (both symmetric and asymmetric) quantum codes. Codes of improved parameters, including many optimal or almost optimal ones, have been obtained through these constructions.

Consensus-based Robust Distributed Estimation

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Abstract. The talk will discuss recent advances in the theory of distributed estimation arising in complex interconnected sensor networks. It will focus on problems of guaranteed performance and robustness of estimator networks in the face of degrading effects of modeling uncertainty and communication disturbances. We will present a novel approach to address these problems using ideas of multiagent consensus and cooperation, through optimization of a so-called transient H-infinity disagreement metric.

Guaranteed Non-quadratic Performance for Quantum Systems with Nonlinear Uncertainties

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Abstract. This paper presents a robust performance analysis result for a class of uncertain quantum systems containing sector bounded nonlinearities arising from perturbations to the system Hamiltonian. An LMI condition is given for calculating a guaranteed upper bound on a non-quadratic cost function. This result is illustrated with an example involving a Josephson junction in an electromagnetic cavity.

Learning the Optimal Image Denoising Model Using Bilevel Optimization

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Abstract. A key issue in image denoising, and in inverse problems as a whole, is the correct choice of data priors and fidelity terms. Depending on this choice, different results are obtained.

Several strategies, both heuristic (dictated by the physics behind the acquisition process) and statistically grounded (e.g. by estimating or learning noise and structure in the data), have been considered in the literature.

Recent approaches in the community also propose to learn the model and the parameter choice by bilevel optimisation techniques. In this talk we propose a PDE-constrained optimization approach for the determination of noise distribution in - exemplarily - total variation (TV) image denoising. A bilevel optimization problem for the determination of the weights correspondent to different types of noise distributions is stated and existence of an optimal solution is proved. A tailored regularization approach for the approximation of the optimal parameter values is proposed thereafter and its consistency studied. Additionally, the differentiability of the solution operator is proved and an optimality system characterizing the optimal solutions of each regularized problem is derived. The optimal parameter values are numerically computed by using a quasi-Newton method, together with semismooth Newton type algorithms for the solution of the TV-subproblems.

Extensions of this method to determining the optimal Generalised TV (GTV) regulariser are discussed. The talk is furnished with TV and GTV denoising examples for MRI images, Poisson corrupted data and the removal of impulse noise.

Decoherence-free linear quantum subsystems

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Abstract. In the talk I show a general theory for characterizing and constructing a decoherence-free (DF) subsystem for an infinite dimensional linear open quantum system. The main idea is that, based on the Heisenberg picture of the dynamics rather than the commonly-taken Schrodinger picture, the notions of controllability and observability in control theory are employed to characterize a DF subsystem. A particularly useful result is a general if and only if condition for a linear system to have a DF component; this condition is used to demonstrate how to actually construct a DF dynamics in some specific examples.

Combustion Instability in Liquid Rocket Engine, Scramjet Engine and SI Engine

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Abstract. In view of engine engineering, combustion instability are widely presented in many engines, such as liquid rocket engine, solid rocket motor, ramjet engine, scramjet engine and SI (spark-ignition) engine (gasoline engines), which is harmful to normal operation of engines and even damage the engine in an instant. In view of combustion techniques, jet flow, mixing layer flow, flow over a backward-facing step and swirling flow are usually applied for purpose of stable ignition and combustion, however combustion instability can be excited in these reacting flows under some extreme conditions. In view of flame itself, there is intrinsic flame instability which may lead combustion instability in engine and real reacting flows. Though combustion instability widely occurs in engine and combustors, its mechanisms and the influences of related factors on it are still not well understanding.

In this paper, three kinds of combustion instabilities are presented. One is high-frequency acoustic combustion instability in model chamber of Lox/RP-1 liquid rocket engine. The predicted peak frequency of pressure oscillation is well agreement with the test. It is found that the premixed gases of fuel and oxygen are rapidly formed due to instant evaporation of fuel droplet when its temperature closes to the critical temperature. Quasi-constant volume combustion happens as soon as such premixed gases formed, and a region with extreme high pressure as well as pressure oscillation with high amplitude therefore appears. The other combustion instability occurs in supersonic reacting mixing layer flows of diluted hydrogen and air. When the temperature of air stream is not high enough for a quick ignition and not low enough for a long-distance ignition, the reacting flows are ignited much later than the turbulent vortex shedding and thus premixed mixtures of fuel and oxidizer are formed accompanying with the vortex entraining. Auto-ignition happens for these premixed mixtures, which is nearly constant-volume combustion and leads to a sharply increase of pressure, temperature and production as well as huge consumption of reactant. Finally, such local extremely high pressure leads combustion instability. It can be concluded that such combustion instability in the supersonic reacting mixing layer is induced by turbulent vortex. The last combustion instability presented in this paper appears in SI engine known as knocking. The pressure oscillation in modeled cylinder is predicted and is consistent with the experimental observations. Such combustion instability is induced by interaction of propagating flames as well as interaction of these propagating flames and pressure waves. Combustion instability is characterized by large-amplitude pressure oscillation in combustor, but it is a very complex phenomenon. As shown in above, the combustion instability happened in different engine or reacting flows may be induced by completely different mechanism.

Contributed Talks

Trapped Modes around Freely Floating Bodies in Two Layer Fluids

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Abstract. We consider a spectral problem that describes the time-harmonic motion of the mechanical system consisting of a three-dimensional rigid body freely floating in a two-layer fluid channel. Unlike the trapping of water waves by fixed obstacles, the interaction of time-harmonic waves with freely floating objects gives rise to a quadratic operator pencil. Under symmetry assumptions in the geometry of the fluid domain, we use a simplified reduction scheme that reduces the quadratic pencil to a linear spectral problem (linear pencil) for a self-adjoint operator in a Hilbert space and we derive a sufficient condition for the nonemptiness of its discrete spectrum. Some examples of floating bodies supporting trapped modes are given.

Properties of the Parameter Space for a Chemotaxis Model

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Abstract. We consider the chemotaxis model based on the equation pair

$$\frac{\partial n}{\partial t} = D\nabla^2 n -- \alpha\nabla.(n\nabla c) + sr(Nn -- n^2), \frac{\partial c}{\partial t} = \nabla^2 c -- sc + s\frac{n}{1+n},$$

where $n = n(x, t)$ denotes cell density at x and at time t and $c = c(x, t)$ denotes the concentration of the chemical attractant. This is a well-known simplification of the Keller-Segel model (3). It has been studied as a more approachable version which is also of interest. In (1), (2) and (5) researchers have developed general results for simplified versions of this pair. Also in (5) Murray simulated the pair and showed how it contains enough variability to model color patterns on reptiles. In that case the simulation method was FDM. Hence, it was restricted to regular partitions of rectangular domains.

Recently we have shown how collocation may be used to simulate the pair. The procedure allows for fast simulation on small computers. Moreover, as these simulations are based on triangular partitions, the simulation domain is no longer restricted. In particular we have used a disk for this analysis of the parameter space.

The parameters are:
D the diffusion parameter, r the mitosis rate,

α the effectiveness parameter,
s the wave number.

It is easy to see that s is the wave number for the initial state of the chemical attractant. Values of s arise from solutions of the Helmholtz equation. Different values of s change the geometry of the resulting cell density pattern but have little effect on the process itself.

We have considered two cases for the remaining parameters. First it is reasonable to consider the diffusion rate as a function of the mitosis rate. Indeed other researchers have made this simplifying assumption. In this case the resulting space is two dimensional. Finally, we consider the full three dimensional parameter space. With D and r fixed, changes in α speed or retard the process. The parameter r has a negative effect. Finally, the process is remarkably stable.

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Moment Methods for the Vlasov-Maxwell Equations

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Abstract. In this talk, we derive the extended magnetohydrodynamic models based on the moment closure of the Vlasov-Maxwell equations. We adopt the Grad type moment expansion which was firstly proposed in 1949 for the Boltzmann equation. A new regularization method for the Grad's moment system of the Boltzmann equation was recently proposed to achieve the globally hyperbolicity so that the local well-posedness of the moment system is attained. For the Vlasov-Maxwell equations, the moment expansion of the convection term is exactly the same as that in the Boltzmann equation, thus the new developed regularization applies. The moment expansion of the electromagnetic force term in the Vlasov-Maxwell equations turns to be a linear source term, which can preserve the properties of the distribution function in the Vlasov-Maxwell equations perfectly.

On Diagonal Stability Analysis of Switched Systems

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Abstract. In this paper we consider the diagonal stability properties of a class of switched linear systems. We present necessary and sufficient condition for the existence of diagonal Lyapunov function for such switched systems using secant criterion. Some examples are also given to illustrate the theoretical results.

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Cartesian Grid Method for the Compressible Navier-Stokes Equations Using Simplified Ghost Point Treatment at Embedded Boundaries

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Abstract. A Cartesian grid method has been developed for solving the 2D compressible Navier-Stokes equations. We introduce two new approaches called the simplified and the modified simplified ghost point treatments for viscous flow near embedded boundaries. These ghost point treatments are already implemented for the 2D compressible Euler equations (1). In these approaches if the wall boundary is in the middle between fluid and ghost points then these approaches are second order accurate for second order schemes. We assign values to the ghost points near solid embedded boundaries from mirror points in the fluid domain to reflect the presence of the solid boundaries. Wall boundary conditions are imposed at the ghost points of the embedded boundary. Accuracy of the Cartesian grid method has been investigated for different test cases. The simplified ghost point treatment is tested for supersonic flow over a circular cylinder. In this test case, the skin friction profiles have been used to assess the accuracy of the Cartesian grid method. We also simulate supersonic viscous flow around NACA0012 airfoil. The lift and drag coefficients along with the pressure coefficients profile are compared with the literature. Although, we found a good agreement between the results of the simplified ghost point treatments but some of the related issues will be discussed in the paper.

Reference

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Large Eddy Simulation of Natural Gas Leakage in Urban Street Canyons

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Abstract. Natural gas leakage in urban street canyons is investigated numerically using large eddy simulation in this paper. At first, in order to verify the numerical method, simulations on flow field and gas dispersion in a model of street canyon in the wind tunnel (1) were carried out. In experiments, two blocks of wood spanning the width of the wind tunnel were used to model the street canyon. An isolated street without other buildings around was chosen to focus on the nature of the flow and gas dispersion inside the street. In the non-isolated street canyon configuration, a third building was added upstream of the street to investigate the influence of a canyon placed in the middle of an urban environment. For the non-isolated street canyon, the computational domain was taken to be 1.2m*0.1m*0.21m, the width of the street canyon was 30 mm, and the heights of buildings near the streets were 30 mm and 50 mm, respectively. Reasonable sub-grid scale model constant and appropriate grid system were determined for simulating gas dispersion in the above mentioned model street canyon. Simulation results showed that there were complicated recirculation flow patterns in the street canyons and in the region of downstream building. Predicted results are in good agreement with the experimental data. Then, numerical investigations on natural gas leakage in a large non-isolated urban street canyons were carried out. The computational domain was taken to be 1200m*100m*210m, the width of the street canyon was 30 m, and the heights of buildings near the streets were 30 m and 50 m, respectively. The principal parameters investigated are wind speed and natural gas leakage intensity. For natural gas leakage, with the wind speed increasing, the natural gas dispersion region within the street canyon increases due to the formed recirculation zone, but the concentrations of natural gas outside the street canyon are reduced due to the blow off effect. With the natural gas leakage intensity increasing, the high natural gas concentration regions within and outside the street canyon increase. For natural gas leakage in urban street canyons, the dangerous regions were analyzed according to the explosive limits of the mixture of natural gas and air. The simulation results are useful for the risk analysis of natural gas leakage.

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An Eulerian Approach of Particle Phase Based on Jordan Decomposition for Compressible Multiphase Flow

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Abstract. Compressible multiphase flow involving gas and particles is studied numerically in this paper. The governing conservation formed equations of the gas phase and the particle phase are both expressed in Eulerian coordinate. For the governing equations of the gas phase, the partial derivatives of the vector fluxes with respect to the vector of conserved variables define the Jacobian matrix. Applying the chain rule to the second term in the Euler equations, the conservation laws can be written in quasi-linear form with the Jacobian matrix representing the coefficient, which is remarkably similar with the inviscid Brugers equation. While the gas is taken to comply with the ideal-gas law, the Euler equations of compressible fluid flow reduce to a strongly hyperbolic system. Therefore, the Jacobian matrix is assumed to be decomposed into an invertible characteristic matrix and a diagonal matrix assembling real numbers which are so-called eigenvalues of the system. The eigenvalues imply the characteristic directions, in which the characteristic parameters in terms of the original variables maintain constant, providing a way of solving the Riemann problem. Compared with the Jacobian matrix of the Euler equations of the gas phase, the particle Euler equation system is not strongly hyperbolic, this indicates that the corresponding coefficient matrix can not be diagonalized. However, considering the fact that spatial differencing is carried out using mesh points on the side from which information flows, in order to apply the upstream scheme to Euler equations of particle phase for performing the discretization procedure, it is important to find out the characteristic direction of the wave propagation speed in the partial differential equations of the particle phase. Instead of diagonalization used for the gas phase, Jordan decomposition for Euler equations of the particle phase is proposed according to the properties of its coefficient matrix. After the decomposition, an invertible matrix can also be obtained along with a Jordan matrix corresponding to the diagonal matrix resulting from Euler equations of the gas phase. The Euler equations of the particle phase are then easily transformed to characteristic equations, in which the signs of the diagonal values of the Jordan matrix are observed to reveal the characteristic directions. As a result, the upstream scheme is available for solving the partial differential equations governing the motions of compressible multiphase flow. For numerical treatment of the equations, the inviscid flux is discretized by Roe-type Riemann solver, and the second-order spatial accuracy is obtained by MUSCL-type scheme. A two-step Runge-Kutta method is used to integrate the equations temporally. The gas and particle motion is regarded as inviscid, so that the fluid viscosity and conductivity are ignored except for the modeling of momentum and thermal interactions between the gas phase and the particle phase.

The proposed Eulerian approach of particle phase is used for calculating compressible gas-particle flow in a shock tube. Apart from the conventional quasi-steady force, the pressure gradient force, the added mass force and the viscous-unsteady force are also taken into account for instantaneous drag modeling. The predicted results show good agreement with the experimental data. Different contributions to the overall forces exerted on the particles are evaluated during the interaction between the gas phase and the particle phase. It is found that the unsteady forces are quite large in the initial period when the shock wave propagates over the particles, and decay very quickly as the time passes on. The reflected and transmitted shock waves caused by the approaching shock encountering the particle phase are also presented in this paper.

Symmetry Transformations and New Explicit Solutions of Two $(2+1)$-Dimensional Differential-Difference Equations

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Abstract. With the aid of Maple, we obtain the symmetry transformations of two (2+1)-dimensional differential-difference equations with the direct method that is extended from the continuous differential equations to the differential-difference equations. Moreover, some new soliton-like solutions and periodic-like solutions of the two differential-difference equations are presented based on the symmetry transformations.

Improving Approximate Singular Triplets in Lanczos Bidiagonalization Method

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Abstract. The singular value decomposition (SVD) of a matrix $A \in R^{m \times N}$ (We assume that $M \geq N$, otherwise, we work on A^T) is

$$A = U\Sigma V^T,$$

where $\Sigma = diag(\sigma_1, \sigma_2, \cdots, \sigma_N)$, $U = (u_1, u_2, \cdots, u_M$ and $V = (v_1, v_2, \cdots, v_N)$ are orthogonal matrices of order M and N, respectively. (σ_i, u_i, v_i) are called the singular triplets of A.

The SVD method is used in many applications, such as determination of numerical rank, least squares problems, image and signal processing, information retrieval, pattern recognition, and so on.

The Lanczos bidiagonalization type methods are the most popular methods for computing few largest and/or smallest singular triplets of large matrices. The main idea of these methods is: after m-step Lanczos bidiagonalization process

$$AQ_m = P_m B_m, A^T P_m = Q_m B_m^T + \beta_{m+1} q_{m+1} e_m^T$$

with P_m and (Q_m, q_{m+1}) be column orthogonal and B_m be upper bidiagonal, the desired singular triplets are extracted from the subspace $span\{P_m\}$ and $span\{Q_m\}$ in different ways.

So, although q_{m+1} has been in hand, it has no contribution for computing the approximate singular triplets. In this talk, we show how to improve the approximate singular triplets by using the information of q_{m+1}.

Effects of Mixture Ratio on Combustion Instability in a RP-1/Lox Rocket Engine

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Abstract. To investigate the effects of the mixture ratio on the combustion instability, a comprehensive code is developed to describe three dimensional transient turbulent two-phase Reacting flow in the chamber of RP-1/Lox liquid rocket engine in this paper. The axial pressure and the axial velocity are qualitative agreement with experimental data. The combustion instability encountered without any disturbance in the initial and boundary conditions. Mixture ratio plays an important role in the spray combustion which affects the combustion instability. Four different mixture ratios in the initial conditions are displayed by changing the mass flow rate of RP-1 or Lox while the total mass flow rate keeps constant in this work. It shows that the smaller mixture ratio in the computed range is benefit to combustion stability. It is hard to form the explosive mixtures in the head of the liquid rocket engine in smaller mixture ratio conditions because of the poor mixing. Hence, mixture ratio is a key factor to combustion instability.

Numerical Simulation of Unsteady Magneto-Hydrodynamic Micropolar Squeeze Film Flow between Parallel Plates

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Abstract. In present paper, the unsteady squeezing hydrodynamics of a magneto-micropolar lubricant between two parallel plates is investigated, in the presence of a uniform strength magnetic field.

The electrically-conducting micropolar constitutive model i.e. magneto-micropolar non-Newtonian fluid model is implemented in this study. In micropolar fluid dynamics, the classical continuum and thermodynamics laws are extended with additional equations which account for the conservation of micro-inertia moments and the balance of first stress moments which arise due to the consideration of micro-structure in a fluid. Hence new kinematic variables (gyration tensor, microinertia moment tensor), and concepts of body moments, stress moments and microstress are combined with classical continuum fluid dynamics theory. The partial differential equations describing the two-dimensional flow regime are transformed into non-dimensional, non-linear coupled ordinary differential equations for linear and angular momentum (micro-inertia). These equations are solved using the robust EFGM (Element Free Galerkin Method). EFGM has been shown to be a very powerful and efficient technique in developing numerical solutions to

strongly nonlinear tribiological flows. The influence of magnetic field parameter (Ha), Eringen vortex viscosity parameter (R), and unsteadiness parameter (S) on linear and angular velocity (micro-rotation) and couple stresses are discussed. Obtained results indicate that increasing magnetic field serves to decelerate the linear velocity and enhance angular velocity of the squeezing flow between the plates. Hence, magnetic field can be used to enhance the lubrication.

Micropolar fluids can accurately simulate physiological fluids consisting of randomly orientated particles suspended in a viscous medium. The present study has immediate applications in medical prosthetics e.g. knee actuators. Such systems can benefit immensely in performance from using rheological fluids which respond to a magnetic field to enhance control.

Modeling of Non Catalytic Tubular Reactor: Flow of Non-Newtonian Fluids under Non-Isothermal Conditions

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Abstract. Tubular reactors are widely used in continuous process industries handling large amount of reactants and products. Also added complexities are thrown in by accompanied heat effects and non Newtonian behavior of the fluids being handled in these reactors. Modeling and experimental studies on simpler reactions involving Newtonian fluids abound in literature but studies pertaining to non- Newtonian fluids are few. So the present study is an important step in this direction as vast majority of reactions involved in polymer processing, food processing, biochemical industries etc. are typical examples of non-Newtonian behavior. Also modeling study of these systems has its obvious advantages compared to elaborate experimentation.

In the present work the modeling and simulation is carried out for the case of non-Newtonian fluids undergoing endothermic reactions in non catalytic tubular reactors with radial dispersion following for Ostwald-de-Waele power law model. The coupled mass balance, energy balance and velocity equations have been formulated and numerically solved using finite difference technique. The effect of variation in the dimensionless parameters obtained from the model has been studied on reactor performance. The analysis of results reveal that, the rheological parameter 'n' has a bearing on the reactor performance. With the increase in 'n' greater velocity distortion and a corresponding decrease in conversion and temperature is observed.

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Applications of Stochastic Separation Flow Model in Numerical Simulation of Supersonic Boundary Layer Flows

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Abstract. In this paper, stochastic separation flow (SSF) models were applied to simulate supersonic particle-laden turbulent flows. The statistical flow field of a supersonic spatially developing boundary layer was supplied by a DNS database. The discrete particles were released continuously from a round hole on the boundary into the mainstream and tracked by means of the SSF, ISSF and TSSSF models. The particle-phase statistics were obtained by a secondary-order time-weighed Eulerian method. The ability of those SSF models were then compared for predicting particle-phase variables including mean and fluctuating velocities, and particle spatial dispersion. For obtaining the stationary and smooth statistical results, the SSF model required a large number of tracked particles, whereas the ISSF model needed the least and the TSSSF model lay in-between. The ISSF model was less predictable for the particle spatial dispersion. Furthermore, the SSF and TSSSF models could better predict the particle transports of boundary layer turbulence. Three models could well predict the mean and fluctuating velocities of particle-phase. The present study is valuable for selecting a proper SSF model for simulating particle-laden turbulent boundary layer flows.

Painlevé Test of the Generalized Variable Coefficient KdV Equation

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Abstract. In this paper, free surface wave equation with variable water depth is studied, the nonlinear transformation is introduced into the KdV equation with space dependent coefficients and then the generalized variable coefficient KdV equation is obtained. By using WTC method, Painlev? properties of the generalized variable coefficients KdV equation are studied, discuss conditions that the variable coefficients KdV equation is integrable .

Tomographic Image Reconstruction with Contourlet Transform

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Abstract. Tomography is a non-invasive technique to see inside an object without opening it up.In Computerized Tomography(CT),cross-section of a human body or a non-destructive object is reconstructed by passing a thin X-ray beam and intensity loss, which defines attenuation coefficient, is recorded by detectors. These measured data is called as Radon Transform, which was introduced by J.Radon in 1917, estimates the intensity loss as average of density function of tissue over hyperplanes. In the image reconstruction for a two dimensional density function $f(x,y)$, Radon Transform is defined by line integrals as

$$g(p,\theta) = \int_{-\infty}^{\infty}\int_{-\infty}^{\infty} f(x,y)\delta(x\cos\theta + y\sin\theta - p)dxdy$$

In any even direction radon transform is not local, i.e. we require all the projections for any fixed point of an image.Thus an approximate inversion formula accomplished by filtered Back-projection algorithm is not local.Many wavelet based inversion formula has been proposed to recover the tomographic images in local region. For one dimensional signal wavelet transform is a good transform and for two dimension it defines discontinuity along edge points only but not visualize the smoothness along curve. Contourlet Transform was first introduced by Do and Vetterli.In the present script, we proposed an reconstruction algorithm with Contourlet transform.Contourlet Transform has a double filter bank structure which defines both localization and directionality.A modified Convolution Backprojection reconstruction algorithm based on Contourlet Transform is proposed, which estimates the image in all the directions using only local measurements. The proposed method calculates the contourlet coefficient of reconstruction image with same complexity as the conventional Convolution Backprojection algorithm.Further we present error estimation for this algorithm and show that it converges faster then other approaches.

A Structured Grid Method for the Singularly Perturbed Reaction-Diffusion Equation from Computational Cardiology

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Abstract. The monodomain equation in computational cardiology, which describes the electrical activity of the heart, is a singularly perturbed reaction-diffusion equation. In this talk, I will introduce a structured grid method for solving the problem. The method applies the technique of operator splitting to integrate the linear diffusion part separately from the nonlinear reaction part. The split linear diffusion equation is solved with the recently developed kernel-free boundary integral method on a Cartesian grid, which does not need to know the kernel of the boundary and volume integrals involved, while the split diffusion equation on a

Cartesian grid itself is a stiff problem and integrated with an L-stable second-order accurate time integration method, called the composite backward differentiation formula. Numerical results for the problem in both two and three space dimensions will be presented. To the best of my knowledge, this is the first Cartesian/structured grid based method for singularly perturbed reaction-diffusion equations (In the literature, there are structure grid based methods for parabolic PDEs but not for singularly perturbed reaction-diffusion equations).

The Effect of Convective Mach Number on The Scalar Dissipation Rate in Supersonic Mixing Layers

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Abstract. As the increasing importance of supersonic combustion, there has been a renewed interest in supersonic mixing layer flows. The residence time of flows in the supersonic combustor is very short. As a result, the mixing of air and fuel and their ignition problem becomes extremely important for the designing of supersonic combustors. Supersonic mixing layer flow which involves two parallel streams is an ideal model for the study of supersonic combustion problems. In this paper supersonic mixing layers has been simulated using a fifth-order conservative hybrid compact-WENO scheme which has been validated in our previous work. Time integration is performed using three-step Runge-Kutta method. The viscous terms is solved by a sixth-order central compact finite difference scheme. In turbulent reacting flows scalar dissipation rate is important for understanding the influence of turbulence on combustion. The statistics of scalar dissipation rate are related to many phenomena such as auto-ignition, the extinction of flame and release of pollutants. It is found that the extinction of flame exists in regions with high values of scalar dissipation rate in non-premixed combustion. Besides, auto-ignition generally takes place in regions with low values of scalar dissipation rate. In this paper we have studied three supersonic mixing layers with convective Mach number as 0.2, 0.6 and 0.8 respectively. It is found that the maximum value of Renolds averaged turbulent kinetic energy is increased with convective Mach number. Furthermore, the statistics of scalar dissipation rate are examined. For the case with convective Mach number as 0.2 and 0.6 the profiles of Renolds averaged scalar dissipation rate are shown with evidently double-peak feature, while for the case with convective Mach number as 0.8 there only one peak in the profile of Renolds averaged scalar dissipation rate. Most importantly, results show that the mixture fraction conditioned scalar dissipation rate is influenced by convective Mach number greatly. Especially when mixture fraction approaches the value of 0.1 and 0.9, the value of conditioned scalar dissipation rate gets much larger as convective Mach number increases. This suggests that it becomes more difficult for ignition with the increase of convective Mach number.

Qualitative Analysis for Boundary Value Problem of a Class of Second-Order Ordinary Differential Equations

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Abstract. In this paper, we research the BVP of a class of nonlinear ordinary differential equations which forms are as follows

$$\frac{d\sigma_{11}}{dr} + \frac{1}{r}(\sigma_{11} - \sigma_{22}) = 0,$$

where $\lambda_1 = -dr/dR$, $\lambda_2 = r/R$, $\lambda_3 = \lambda$ are the principal stretches; the principal Cauchy stresses are $\sigma_{ii} = \lambda_i W_i/J$, $W_i = \partial W/\partial\lambda_i, i = 1, 2, 3; J = \lambda_1\lambda_2\lambda_3; W = W(\lambda_1, \lambda_2, \lambda_3)$ is the strain-energy function associated with a certain compressible hyperelastic material. Here we consider the following strain energy densities for compressible materials

$$W = C_1(j_1 - 3) + C_2(j_2 - 3)C_3(j_3 - 1),$$

where C_1, C_2, and C_3 are material constants, j_1, j_2 and j_3 are the invariants of the stretch tensor.

The boundary conditions and the end condition are proposed by

$$\sigma_{11}(a) = \sigma_{11}(b) = 0,$$

$$N = 2\pi \int_a^b r\sigma_{33}dr = 0.$$

where $r(A) = b, r(B) = a; A \leq R \leq B, a \leq r \leq b.$

The above BVP can been used to describe the eversion problem of a class of compressible hyperelastic thin-walled cylindrical tubes. However, the exact solution of the problem is not available. Numerical simulations allow us to deduce the qualitative behavior of the solution and then the relations among axial stretch rate, initial thickness and inner (outer) radius are obtained. The effects of the material parameter and the structure parameter on the finite deformation of the compressible hyperelastic thin-walled cylindrical tubes are discussed.

The Interaction between Flame and Aerodynamic Waves in One-Dimensional Confined Space

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Abstract. The energy and environmental pollution problem has become one of the most important problems nowadays. One useful and practical way to ease the problem is to develop higher efficiency, clear gasoline engine. It can be possibly achieved by increasing the compression ratio, yet this also makes the 'knock' phenomenon more easily to occur, resulting in possible damage of the engine. To solve the knock problem, which has been investigated widely but still not understood thoroughly, further study about its underlying physical mechanisms is needed.

In the present study, a simplified numerical model is employed to simulate the combustion process in confined space to study the knock phenomenon, which is characterized by rapid pressure oscillations. The simulation was carried out on a one-dimensional confined space domain, using H_2/O_2 with equivalent ratio of 1.0 as premixed combustible mixture, which is ignited by a preset initial hot thin layer attaching to one of the end walls. The detailed reaction mechanism, governing equations for one-dimensional compressible reactive flow with turbulent effect neglected, and adaptive grid technique are employed.

In the simulation results, the phenomenon of rapid pressure oscillations was observed; meanwhile, the interactions between the flame, aerodynamic waves, and the two end walls make the flame propagation process very complex, however some kind of periodical regularity in the flame-aerodynamic wave interaction processes is observed, which is thought to be responsible for the triggering of the rapid pressure vibrations. For example, when a shock coming from the unburnt side hits the flame, it may produce a transmitted shock and reflected wave, and the burning intensity during collision shows no large variation; however, when a shock from the burnt side hits the flame, it may produce a considerably strengthened transmitted shock and reflected wave, and the burning intensity is increased rapidly during collision. These periodically occurred flame-aerodynamic wave interactions result in the final rapid pressure oscillation.

Comparison of the simulation results with experimental results was also made. Comparisons of some important global characters of the flame propagation process, i.e. the average absolute speed of the flame front, the aerodynamic wave structure in the confined space, and the history of pressure variations at two certain points, have shown good qualitative agreement, with some quantitative deviation mainly caused by the two dimensional effects in experiments.

Stream 2
Computational Optimization

Invited Talks

A Two-stage Image Segmentation Method using a Convex Variant of the Mumford-Shah Model and Thresholding

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Abstract. The Mumford-Shah model is one of the most important image segmentation models, and has been studied extensively in the last twenty years. In this talk, we propose a two-stage segmentation method based on the Mumford-Shah model. The first stage of our method is to find a smooth solution g to a convex variant of the Mumford-Shah model. Once g is obtained, then in the second stage, the segmentation is done by thresholding g into different phases. The thresholds can be given by the users or can be obtained automatically using any clustering methods. Because of the convexity of the model, g can be solved efficiently by techniques like the split-Bregman algorithm or the Chambolle-Pock method. We prove that our method is convergent and the solution g is always unique. In our method, there is no need to specify the number of segments K ($K \geq 2$) before finding g. We can obtain any K-phase segmentations by choosing $(K-1)$ thresholds after g is found in the first stage; and in the second stage there is no need to recompute g if the thresholds are changed to reveal different segmentation features in the image. Experimental results show that our two-stage method performs better than many standard two-phase or multi-phase segmentation methods for very general images, including anti-mass, tubular, MRI, noisy, and blurry images.

Unconstrained Optimization Models for Computing Several Extreme Eigenpairs of Real Symmetric Matrices

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Abstract. This paper considers the problem of computing several extreme eigenpairs of real symmetric ma- trices. Based on the variational principles, we put forward some new unconstrained models for this classical problem and further analyze some significant properties. It is shown that the extreme eigen- pairs of any real symmetric matrix can be recovered from the global minimizers of our unconstrained quartic and β-order models. The alternate Barzilai-Borwein method with the adaptive nonmonotone line search is then utilized for solving the

unconstrained models. The preliminary numerical results indicate that our approach is promising.

This is a joint work with Bo Jiang and Chunfeng Cui.

A Smooth Path-Following Approach to the Determination of a Perfect and d-proper Equilibrium

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Abstract. To overcome the numerical instability of Myersons proper refinement of Nash equilibrium, this paper first introduces the concept of perfect and d-proper equilibrium, whose degree of properness is determined by the value of d. Then an interior-point path-following method is developed to determine a perfect and d-proper equilibrium of a finite n-person game in normal form. The basic idea of the method is to closely approximate Nash equilibrium of a perturbed game by incorporating a barrier term into each player's payoff function with an appropriate convex combination. A desired property of multilinear form of the payoff function and an application of the problem's differentiability ensures the existence of a smooth path that starts from a totally mixed strategy profile and ends at a perfect and d-proper equilibrium. A predictor-corrector method is adopted for following the path. Numerical results further confirm the effectiveness of the method.

Beamforming for Problems with Discrete Antenna Weights

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Abstract. Beamforming techniques can be used to increase the throughput of a wireless link as well as to decrease its energy consumption. For such purposes, depending on the kind of antennas, these techniques enable to adjust the beam including its direction in a certain range. We concentrate on antennas formed by an array of single antenna elements. The signal received or transmitted by an antenna array is a weighted complex sum of the signals (amplitude and phase) of each antenna element. In contrast to many existing works for optimizing the antenna weights of the elements we assume that, due to technological reasons, the weights can only range in a discrete set. Therefore, any optimization model to adjust the beam contains integer variables. The number of integer points growth with the number of antenna elements and that of the complex discrete weights. Thus, the solution of such a problem can be very challenging. We focus on beamforming models for a receive antenna with the aim to maximize the Signal-to-Interference-plus-Noise-Ratio (SINR). To this end, we present approaches that are based on the branch-and-bound principle. In particular, both for an approximate and an exact SINR-maximization model we show how inexpensive lower bounds for the objective can be obtained. Moreover, we present computational results and give an outlook to other related models.

Calibration of a New Density-Dependent Flow Model with Implicit Filtering

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Abstract. In this talk we show how implicit filtering can be used to calibrate a new model of density-dependent flow through porous media. The motivating application is salt water intrusion into coastal aquifers, a significant problem in North Carolina. The model is a highly nonlinear DAE-PDE for fluid pressure and mass fraction. We have a large amount of experimental data, and calibrate the model with a standard nonlinear least squares formulation.

While differentiable in its parameters, the numerical implementation of the model can (and does) fail for some parameter values. These failures and the difficulties in differentiating analytically a constantly changing model motivate a derivative-free approach.

Implicit filtering is a derivative-free algorithm which is able to handle failures. For nonlinear least squares problems implicit filtering combines a direct search with a finite-difference damped Gauss-Newton or Levenberg-Marquardt iteration.

We will describe the model, the experiments, the numerics, implicit filtering, and the results of the calibration in this talk.

Exploiting Nonlinear Structure in Mixed-Integer Nonlinear Optimization

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Abstract. Many important design problems involve not only continuous variables with nonlinear relationships but also discrete decisions, giving rise to mixed-integer nonlinear programming problems (MINLPs). MINLPs combine the combinatorial complexity of the discrete decisions with the numerical challenges of the nonlinear and nonconvex functions, giving rise to tough global optimization problems. Applications of MINLP include the modeling of the power grid for network expansion or transmission switching, the optimal reloading of nuclear reactors, the optimal response to oil-spill disasters, and the design of nano-photonic divides.

We will review existing methods for solving MINLPs and present a new package for solving mixed-integer nonlinear optimization problems, MINOTAUR. The MINOTAUR toolkit is designed to provide a flexible and efficient framework for solving MINLPs. We will show how MINOTAUR enables us to exploit nonlinear structure in the solution process. We also present a new approach to generate tight and computationally tractable convex relaxations based on exploiting group-partial separability of the nonlinear functions. We demonstrate this approach in the context of two classes of powerful relaxation techniques: semi-definite relaxations and the reformulation-linearization technique. In both cases, we derive tight relaxations that can be

solved orders of magnitude faster. We conclude with an outlook of the computational challenges and further research opportunities in MINLP.

Randomized Block Coordinate Gradient Methods for a Class of Nonlinear Programming

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Abstract. In this talk we discuss randomized block coordinate gradient (RBCG) methods for minimizing the sum of two functions in which one of them is block separable. In particular, we present new iteration complexity results for these methods when applied to convex optimization problems. We also propose nonmonotone RBCG methods for solving a class of nonconvex problems with the above structure, and establish their global convergence. Finally, we present new complexity results for the accelerated RBCG method proposed by Nesterov for solving unconstrained convex optimization problems.

Penalty Methods with Stochastic Approximation for Stochastic Nonlinear Programming

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Abstract. We propose a unified framework of penalty methods with stochastic approximation for stochastic nonlinear programming.

The worst-case complexity of calls to the stochastic first-order oracle for the proposed methods is analyzed. Moreover, for problems with only stochastic zeroth-order information available, we also propose a penalty method with stochastic approximation for solving the stochastic nonlinear programming. The worst-case complexity of calls to the stochastic zeroth-order oracle is also analyzed.

Numerical Verification of Hyperbolicity for 3-manifolds

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Abstract. For a given cusped 3-manifold M admitting an ideal triangulation, we describe a method to rigorously prove that either M or a filling of M admits a complete hyperbolic structure via verified computer calculations. Central to our method are an implementation of interval arithmetic and Krawczyk's Test. These techniques represent an improvement over existing algorithms as they are faster while accounting for error accumulation in a more direct and user friendly way.

This work is a joint work with Neil Hoffman (University of Melbourne), Kazuhiro Ichihara (Nihon University), Masahide Kashiwagi (Waseda University) Hidetoshi Masai (Tokyo Institute of Technology), and Akitoshi Takayasu (Waseda University)

Stability Optimization for Polynomials and Matrices

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Abstract. Suppose that the coefficients of a monic polynomial or entries of a square matrix depend affinely on parameters, and consider the problem of minimizing the root radius (maximum of the moduli of the roots) or root abscissa (maximum of their real parts) in the polynomial case, or the spectral radius (maximum of the moduli of the eigenvalues) or spectral abscissa (maximum of their real parts) in the matrix case. These functions are not convex and they are typically not locally Lipschitz near minimizers. We first address polynomials, for which some remarkable analytical results are available in one special case, and then consider the more general case of matrices. These root radius and abscissa and spectral radius and abscissa optimization problems arise in many applications, particularly optimizing stability of feedback control systems. We describe several applications, focusing on the static output feedback problem for linear dynamical systems, and present numerical results showing that optimal solutions are typically characterized by multiple roots or multiple eigenvalues.

The polynomial results are joint with V. Blondel, M. Gurbuzbalaban and A. Megretski.

Social Welfare Maximization in Social Media Advertising

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Abstract. We propose a pay-per-forward model for social media advertising. We study the computation and complexity of the optimal allocation. We prove that no adaptive algorithm can find an O(loglogm/logm)-approximate solution using worst-case analysis. In the Bayesian model, we show that the social welfare optimization problem can be formulated as a convex program. A polynomial-time solvable and truthful auction protocol can be derived.

Estimating Dynamic Discrete-Choice Games of Incomplete Information

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Abstract. We investigate the estimation of models of dynamic discrete-choice games of incomplete information, formulating the maximum-likelihood estimation exercise as a constrained optimization problem which can be solved using state-of-the-art constrained optimization solvers. Under the assumption that only one equilibrium is played in the data, our approach avoids repeatedly solving the dynamic game or finding all equilibria for each candidate vector of the structural parameters. We conduct Monte Carlo experiments to investigate the numerical performance and finite-sample properties of the constrained optimization approach for computing the maximum-likelihood estimator, the two-step pseudo maximum-likelihood estimator and the nested pseudo-likelihood estimator, implemented by both the nested pseudo-likelihood algorithm and a modified nested pseudo-likelihood algorithm.

This is joint work with Michael Egesdal and Zhenyu Lai, Harvard University.

Multi-Stage Convex Relaxation Approach for Low-Rank Structured PSD Optimization Problems

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Abstract. This work is concerned with low-rank structured positive semidefinite (PSD) matrix optimization problems. For this class of NP-hard problems, we start from the primal-dual viewpoint to reformulate it as a mathematical program with PSD equilibrium constraints (MPSDEC for short), and show that the penalty version of this MPSDEC, yielded by introducing the complementarity constraint into the objective, is exact in the sense that it has the same global optimal solution set as the MPSDEC problem when the penalty parameter is over a

certain threshold. Then, by solving the exact penalty problem of the MPSDEC in an alternating way, we propose a unified framework for designing the multi-stage convex relaxation approach to the low-rank structured PSD matrix optimization problem. This class of convex relaxation methods solves at each iteration a weighted trace norm minimization problem, which is different from those weighted trace norm minimization problems considered in the literature. For the proposed multi-stage convex relaxation approach, under conditions weaker than the RIP, we establish an error bound for the optimal solution of the kth sub-problem to the global optimal solution, and show that the error bound in the second stage is strictly less than that of the first stage with the reduction rate over 30% for some convex relaxation methods in this framework. In particular, this error bound sequence can be controlled by a strictly decreasing sequence. Numerical results are reported for several classes of low-rank structured PSD matrix recovery, including the low-rank correlation matrix recovery, the low-rank density matrix recovery, and the low-rank Toeplitz matrix recovery, which verify the efficiency of the proposed approach.

This is joint work with Shujun Bi and Shaohua Pan.

Solving Stochastic VI via Expected Residual Minimization

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Abstract. Relying on expected residual minimization, combined with smoothing and sample average approximations is shown to be a potentially effective method to obtain solutions to certain classes of stochastic variational inequalities.

This lecture is based on joint work with X.Chen and Y. Zhang.

First- and Second-Order Necessary Conditions via Exact Penalty Functions

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Abstract. In this paper we study first- and second-order necessary conditions for nonlinear programming problems from the viewpoint of exact penalty functions. By applying the variational description of regular subgradients, we first establish necessary and sufficient conditions for a penalty term to be of KKT-type by using the regular subdifferential of the penalty term. In terms of the kernel of the subderivative of the penalty term, we also present sufficient conditions for a penalty term to be of KKT-type. We then derive a second-order necessary condition by assuming a second-order constraint qualification which requires that the second-order linearized tangent set is included in the closed convex hull of the kernel of the parabolic subderivative of the penalty term. In particular, for an $l_{2/3}$ penalty term, by assuming the nonpositiveness of a

sum of a second-order derivative and a third-order derivative of the original data and applying a third-order Taylor expansion, we obtain the second-order necessary condition.

Smoothing SQP Methods for Solving Nonsmooth and Nonconvex Constrained Optimization Problems

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Abstract. We propose a smoothing sequential quadratic programming (SQP) algorithm for solving a nonsmooth and nonconvex constrained optimization problem. We show that any accumulation point of the iteration sequence generated by the smoothing SQP algorithm is a Clarke stationary point, provided that the sequence of the multipliers and the sequence of exact penalty parameters are bounded. Furthermore, we introduce a new constraint qualification called the weakly generalized Mangasarian Fromovita constraint qualification (WGMFCQ) that is weaker than the GMFCQ. We show that the extended version of the WGMFCQ guarantees the boundedness of the sequence of the multipliers and the sequence of the exact penalty parameters and thus guarantees the global convergence of the smoothing SQP algorithm. We demonstrate that the WGMFCQ can be satisfied by bilevel programs for which the GMFCQ never holds. Preliminary numerical experiments show that our algorithm can be used to solve nonsmooth and nonconvex optimization problems, including the bilevel program.

Complexity Analysis beyond Convex Optimization

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Abstract. A powerful approach to solving difficult optimization problems is convex relaxation. In one application, the problem is first formulated as a cardinality–constrained linear program (LP) or rank-constrained semidefinite program (SDP), where the cardinality or rank corresponds to the target support size or dimension. Then, the non-convex cardinality or rank constraint is either dropped or replaced by a convex surrogate, thus resulting in a convex optimization problem. In this talk, we explore the use of a non-convex surrogate of the cardinality or rank function, namely the so-called Schatten quasi-norm. Although the resulting optimization problem is non-convex, we show, for many cases, that a first and second order KKT or critical point can be approximated to arbitrary accuracy in polynomial time. We also summarize a few complexity analysis results of more general non-convex optimization, which recently becomes a popular research topic and hopefully leads to more effective non-convex optimization solvers.

On the Extension of ADMM for Separable Convex Programming and Beyond: From Variational Inequality Perspective

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Abstract. The alternating direction method of multipliers (ADMM) is now widely used in many fields. It is strongly desired and practically used to extend ADMM naturally to the case of convex programming where its objective function is the sum of three convex functions without coupled variables. The direct extension of ADMM, however, is not necessarily convergent even though it performs verywell for many applications. We propose a prototype algorithm in form of variational inequality for the separable convex minimization model with three uncoupled objective functions. The extended ADMM and some benchmarks in the literature such as the augmented Lagrangian method (ALM) and the original ADMM can all be recovered by this prototype algorithm. A unified and easily checkable condition to ensure the convergence of this prototype algorithm is given. To make this prototype algorithm specific, we propose a class of ADMM-based algorithms that preserve completely the numerical advantages of the extended ADMM. Theoretically, we show the contraction property of the prototype algorithm, and consequently establish its global convergence and worst-case convergence rates measured by iteration complexity. Numerically, an important feature of this new class of algorithms is that they could be even faster than the extended ADMM for some applications.

On the Convergence and Worst-Case Complexity of Trust-Region and Regularization Methods for Unconstrained Optimization

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Abstract. A nonlinear stepsize control framework for unconstrained optimization was recently proposed by Toint (2013), providing a unified setting in which the global convergence can be proved for trust-region algorithms and regularization schemes. The original analysis assumes that the Hessians of the models are uniformly bounded. In this paper, the global convergence of the nonlinear stepsize control algorithm is proved under the assumption that the norm of the Hessians can grow by a constant amount at each iteration. The worst-case complexity is also investigated. The results obtained for unconstrained smooth optimization are extended to some algorithms for composite nonsmooth optimization and unconstrained multiobjective optimization as well.

This is joint work with Geovani N. Grapiglia and Jinyun Yuan.

New Results in Tensor and Polynomial Optimization

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Abstract. In this talk we shall present some recent results for tensor/polynomial optimization problems. Among them, we shall discuss solution methods for the tensor PCA (Principal Component Analysis) problem, which has found wide applications in Magnetic Resonance Imaging (MRI), radar signal processing, DNA expression data analysis, video image data recovery. We shall also discuss tensor co-clustering problems, tensor approximation, and their applications in bioinformatics.

The work presented in this talk is based on joint research projects with: Bilian Chen, Xiuzhen Huang, Bo Jiang, Zhening Li, Shiqian Ma, and Andre Uschmajew.

Contributed Talks

Complexity Analysis of Interior Point Algorithms for Non-Lipschitz and Nonconvex Minimization

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Abstract. We propose a first order interior point algorithm for a class of non-Lipschitz and nonconvex minimization problems with box constraints, which arise from applications in variable selection and regularized optimization. The objective functions of these problems are continuously differentiable typically at interior points of the feasible set. Our first order algorithm is easy to implement and the objective function value is reduced monotonically along the iteration points. We show that the worst-case iteration complexity for finding an ϵ scaled first order stationary point is $O(\epsilon^{-2})$. Furthermore, we develop a second order interior point algorithm using the Hessian matrix, and solve a quadratic program with a ball constraint at each iteration. Although the second order interior point algorithm costs more computational time than that of the first order algorithm in each iteration, its worst-case iteration complexity for finding an ϵ scaled second order stationary point is reduced to $O(\epsilon^{-3/2})$. Note that an ϵ scaled second order stationary point must also be an ϵ scaled first order stationary point.

This is joint work with Xiaojun Chen and Yinyu Ye.

On the Convergence of the Self-Consistent Field Iteration for Solving the Kohn-Sham Equation

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Abstract. It is well known that the self-consistent field (SCF) iteration for solving the Kohn-Sham (KS) equation often fails to converge, yet there is no clear explanation. In this talk, we investigate the SCF iteration from the perspective of minimizing the corresponding KS total energy functional. By analyzing the second-order Taylor expansion of the KS total energy functional and estimating the relationship between the Hamiltonian and the part of the Hessian which is not used in the SCF iteration, we are able to identify some conditions to ensure global convergence from an arbitrary initial point to and local linear convergence from an initial point sufficiently close to the solution of the KS equation. Our analysis holds under mild assumptions that the second-order derivatives of the exchange correlation functional are uniformly bounded from above.

On Solving a Quadratic Programming Problem Involving Distances in Trees in Polynomial Time

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Abstract. Let $G = (V, E)$ be a connected graph with vertex set V and edge set E: Let $c : V(G) \to R_+$ be a nonnegative vertex weight function such that the total weight of the vertices is $N = \sum_{v \in V(G)} c(v)$. Suppose $d_G(u, v)$ denotes the usual distance (the length of the shortest path) between u and v in G. Then the total distance of G with respect to c, is defined by

$$d_c(G) = \sum_{\{u,v\} \subseteq V(G)} c(u)c(v)d_G(u, v).$$

Among all nonnegative weight functions c of given weight N, we seek to find the one which maximizes $d_c(G)$.

Dankelmann [Discrete Mathematics 312 (2012)12-20] considers this problem and it was left as an open problem with remarks that "we do not know if, for all graphs or possibly for a restricted class of graphs such as trees, a weight function maximizing $d_c(G)$ can be found in polynomial time." In this talk, we show that indeed for trees the problem can be solved in polynomial time. This is achieved by converting the problem into a quadratic programming problem with a positive definite matrix.

Besides the graph theory literature, more general versions of this problem have occurred in the literature in different contexts such as a generalized notion of diameter of a finite metric space and Nash equilibria of symmetric bimatrix games. This problem can be processed by Lemke's algorithm.

This is joint work with R. B. Bapat.

Reconstruction of Periodic Binary Matrices from row and column projections by Simulated Annealing

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Abstract. Discrete Tomography (DT) (1) refers to the reconstruction of discrete sets from its projections. Del Lungo et al. (2) studied the DT problem of reconstruction of (p, 1) - periodic binary matrices from their row and column projections. In 2010, Jarray and Tlig (3) presented a Simulated Annealing algorithm for the DT problem of reconstructing hv-convex binary matrices from their row and column sums. We focus on the problem of reconstruction of a periodic binary matrix of a given period (p, q) from its row and column projections. We convert this problem into an optimization problem based on some theoretical results presented. Then we solve this optimization problem by developing a simulated annealing algorithm. Numerical

experiments are carried out on binary matrices of varying orders and periods. Competitive results are obtained.

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Regularized Mathematical Programs with Stochastic Equilibrium Constraints: Estimating Structural Demand Models

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Abstract. The article considers a particular class of optimization problems involving set-valued stochastic equilibrium constraints. A solution procedure is developed by relying on an approximation scheme for the equilibrium constraints, based on regularization, that replaces them by equilibrium constraints involving only single-valued Lipschitz continuous functions. In addition, sampling has the further effect of replacing the 'simplified' equilibrium constraints by more manageable ones obtained by implicitly discretizing the (given) probability measure so as to render the problem computationally tractable. Convergence is obtained by relying, in particular, on the graphical convergence of the approximated equilibrium constraints. The problem of estimating the characteristics of a demand model, a widely studied problem in micro-economics, serves both as motivation and illustration of the regularization and sampling procedure.

Regularization and Smoothing of Differential Variational Inequality with Application to Dynamic Games

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Abstract. Differential variational inequality (DVI) is a new modeling paradigm, which is a system of ordinary differential equations (ODE) subject to a variational inequality with parameters. Solving this problem is challenging because it may involve a family of parameterized optimization problems without standard constraint qualifications. Another difficulty is that the solution of the DVI is usually non-smooth, and because of this we can not expect a high order convergence even when high order ODE-integrators are applied.

In this work we use regularization and smoothing techniques to develop a method for solving the DVI, which is shown convergent to the least norm solution of the DVI as the regularization parameter and the smoothing parameter go to zero. The computational cost of the method is for solving a system of ODEs with boundary value conditions.

We also study applying the method to the dynamic game in generalized form, which involves a dynamic decision process with multiple players, where not only the players' cost functionals but also their admissible control sets depend on the rivals' decision variables through shared constraints. By numerical example, we illustrate that the regularization smoothing method can give an approximation of a Nash equilibrium of the dynamic game.

Sparse Index Tracking based on L1/2 Model and Algorithm

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Abstract. Recently, L1 regularization have been attracted extensive attention and successfully applied in mean-variance portfolio selection for promoting out-of-sample properties and decreasing transaction costs. However, L1 regularization approach is ineffective in promoting sparsity and selecting regularization parameter on index tracking with the budget and no-short selling constraints, since the 1-norm of the asset weights will have a constant value of one. Our recent research on L1/2 regularization has found that the half thresholding algorithm with optimal regularization parameter setting strategy is the fast solver of L1/2 regularization, which can provide the more sparse solution. In this paper we apply L1/2 regularization method to stock index tracking and establish a new sparse index tracking model. A hybrid half thresholding algorithm is proposed for solving the model. Empirical tests of model and algorithm are carried out on the eight data sets from OR-library. The optimal tracking portfolio obtained from the new model and algorithm has lower out-of-sample prediction error and consistency both in-sample and out-of-sample. Moreover, since the automatic regularization parameters are selected for the fixed number of optimal portfolio, our algorithm is a fast solver, especially for the large scale problem.

Gradient Consistency of Smoothing Functions for the Integrable Functions and Applications

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Abstract. We consider smoothing methods for the stochastic optimization problems where the objective function is continuous but not differentiable and defined by the expectation of a random function. This kind of problems arise from wide applications such as stochastic equilibrium, risk measures, finance and so on. We present the gradient consistency of the subdifferential associated with a smoothing function for the integrable function under some suitable conditions. We discuss the applications of the developed theory to the problems of the generalized stochastic Nash games, stochastic variational inequalities and risk measures. We show that conditions and assumptions for this paper hold for these applications.

Optimization Methods for Finding Spherical t_ε-design on the Sphere

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Abstract. Spherical t-design is an equal weight numerical integration quadrature rule with algebraic accuracy degree t. In this report we will study the spherical t_ε-design, which allows the positive weights to perturb in an small interval with respect to a parameter ε. We will reformulate the spherical t_ε-design equations as a nonsmooth and nonconvex optimization problem and propose a smoothing trust region filter algorithm for solving the problem. Numerical results show that the proposed algorithm is effective to solve this problem, comparing with several algorithms and codes including `fmincon, isqnonlin, fsolve` in Matlab. Moreover, numerical results show spherical t_ε-design provides higher algebraic accuracy degree than spherical t-design with same number of points.

Stream 3
Statistical Modeling and Computational Statistics

Invited Talks

On the Bartlett Correction of Empirical Likelihood of Gaussian Long Memory Time Series

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Abstract. Bartlett correction is one of the desirable features of empirical likelihood (EL) since it allows constructions of confience regions with improved coverage probabilities. Previous studies demonstrated the Bartlett correction of EL for independent observations and weakly dependent time series. By establishing the validity of Edgeworth expansion for the signed root empirical log-likelihood ratio, a moderate Bartlett correction of EL for long memory time series is established. In particular, orders of the coverage error of confidence regions can be reduced from $\log^6 n/n$ to $\log^3 n/n$, which is different from the classical rate of reduction from n^{-1} to n^{-2}.

Modeling Clustering Effects of Recurrent Events Using Self-exciting Processes

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Abstract. Semiparametric models of self-exciting processes are proposed for analysis of recurrent events with clustering dependence and illustrated with real examples.

A Constructive Approach to High-Dimensional Linear Regression

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Abstract. We develop a constructive approach to estimating a linear regression model $y = X\beta^\dagger + \eta$ in high-dimensions. The proposed approach is a computational algorithm that generates a sequence of solutions $\{\beta^k, k \geq 1\}$ iteratively, based on support detection using primal and dual information and root finding according to a modified KKT condition for the ℓ_0 penalized least squares criterion. We refer to the proposed algorithm as SDAR for brevity. Under certain regularity conditions on X and sparsity assumption on $\beta^\dagger$, we show that with high probability, $\|\beta^k - \beta^\dagger\|_2$ decays exponentially to $O(\sqrt{\|\beta^\dagger\|_0 \log(p)/n})$ and $\|\beta^k - \beta^\dagger\|_\infty$ decays exponentially to $O(\sigma\sqrt{\log(p)/n})$ when $\eta \sim \mathcal{N}(0, \sigma^2 I_n)$. Moreover, with high probability, it takes no more than $O(\log[\max\{|\beta_i^\dagger||\beta_i^\dagger \neq 0\}/\min\{|\beta_i^\dagger||\beta_i^\dagger \neq 0\}])$ steps to recover the oracle estimator if the minimum magnitude of the nonzero elements of $\beta^\dagger$ is of the order $O(\sigma\sqrt{\log(p)/n})$ for Gaussian noise. We also obtain similar results in the case where $\beta^\dagger$ is not strictly sparse but most of its components are small. Computational complexity analysis shows that the cost of SDAR is $O(np)$ in each step if $\beta^\dagger$ is sparse or can be sparsely approximated. Simulation studies support our theoretical results. We also consider ASDAR, an adaptive version of SDAR to make it more practical in applications. Numerical comparisons with Lasso and MCP indicate that ASDAR is competitive with or outperforms them in accuracy and efficiency.

On the SURE-Type Shrinkage Estimation

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Abstract. The talk is concerned with empirical Bayes shrinkage estimators for the heteroscedastic hierarchical normal model based on Stein's unbiased estimate of risk (SURE). By putting priors for both means and variances, we proposed double-shrinkage SURE type estimators that shrink both the means and the variances. Optimal properties for these estimators were derived. The methods were applied to the well-known baseball data set.

Joint Inference for Competing Risk Data

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Abstract. This research develops joint inferential methods for the cause specific hazard function and the cumulative incidence function of a specific type of failure to assess the effects of a variable on the type of failure of interest in the presence of competing risks. Joint inferences for the two functions should be made routinely in practice because 1) they describe different characteristics of a particular type of failure, 2) they do not uniquely determine each other, and 3) the effects of a variable on the two functions can be different and one often does not know which effects are to be expected. We study both the group comparison problem and the Coxs regression problem. We also develop joint inference for other equivalent pairs of functions. Our simulation shows that the derived joint tests can be considerably more powerful than the Bonferroni method, which has important practical implications to the analysis and design of clinical studies with competing risks data. We illustrate our methods using a Hodgkins disease data and a lymphoma data.

AIC-Type Model Selection Criterion for Longitudinal Data Incorporating GEE Approach

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Abstract. Akaike Information Criterion, which is based on maximum likelihood estimation and cannot be applied directly to the situations when likelihood functions are not available, has been modified for model selection in longitudinal data with generalized estimating equations via working independence model. This paper proposes another modification to AIC, the difference between the quasi-likelihood of a candidate model and of a narrow model plus a penalty term. Such difference avoids calculating complex integration from quasi-likelihood, but inherits theoretical asymptotic properties from AIC. As a by-product, we also give a theoretical justification of the equivalence in distribution between quasi-likelihood ratio test and Wald test incorporating GEE approach. Numerical performance supports its preference to its competitors. The proposed criterion is applied to analyze a real dataset as an illustration.

Estimating a Unitary Effect Summary Based on Combined Survival and Quantitative Outcomes

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Abstract. In practice, when both survival and quantitative outcomes are of interest, we encounter outcomes of mixed types: a censored and a quantitative outcome. Joint modelling of the survival and quantitative outcomes other than analyzing the outcomes separately has become a method of choice for analyzing mixed outcome data because of improved efficiency. However, the joint modeling provides two separate indexes for measuring the covariate (e.g., treatment) effect, making its interpretation difficult when the covariate inconsistently affects the quantitative and survival outcomes. By assigning a single rank to each outcome to represent the disease severity, paper provides a unitary effect summary of the covariates on mixed outcome data while accounting for censoring. The method is applied to an analysis of the AIDS Clinical Trials Group protocol 175 (ACTG 175) data.

This is joint work with Yi Li and Ming T. Tan.

Inference for ARMA Models with Unknown-Form and Heavy-tailed ARCH-type Noises

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Abstract. Recent research reveals that the traditional inference is invalid for the ARMA model with unknown-form and heavy-tailed ARCH-type noises. This paper is to develop a systematic procedure for statistical inference of this model. We first study the Hill's estimator for the tail index and show that this estimator is consistent and asymptotic normal. We then investigates the least absolute deviation (LAD) estimator and the self-weighted LAD estimator for the model. Both estimators are shown to be strongly consistent and asymptotically normal when the noise has a finite variance and infinite variance, respectively. The random weighting approach is proposed for statistical inference under this nonstandard case. We further develop a score-based good-ness-fit test for model adequacy and a Wald test for structural change of models. The limiting distributions of both test statistics are obtained. Simulation study is carried out to access the performance of our procedure and a real example is given to illustrate our procedure.

Nonparametric Estimation of Probability Density Functions for Irregularly Observed Spatial Data

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Abstract. Nonparametric estimation of probability density functions, both marginal and joint densities, is a very useful tool in statistical modelling and computation. The kernel method is popular and applicable to dependent data, including time series and spatial data. But at least for the joint density, one has had to assume that data are observed at regular time intervals or on a regular grid in space. Though this is not very restrictive in the time series case, it often is in the spatial case. In fact, to a large degree it has precluded applications of nonparametric methods to statistical modelling and computation for spatial data because such data often are irregularly positioned over space.

In this paper, we propose nonparametric kernel estimators for both the marginal and in particular the joint probability density functions for non-gridded spatial data. Large sample distributions of the proposed estimators are established under mild conditions, and a new framework of expanding-domain infill asymptotics is suggested to overcome the shortcomings of spatial asymptotics in the existing literature. A practical, reasonable selection of the bandwidths on the basis of cross-validation is also proposed. We illustrate by both simulations and real data examples of moderate sample size that the proposed methodology is effective and useful in uncovering nonlinear spatial dependence for general, including non-Gaussian, distributions.

This is a joint work with Dag Tjostheim. The financial supports from the Australian Research Councils Discovery Project and Future Fellowships grants are acknowledged.

Contrasted Penalized Integrative Analysis

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Abstract. Single-dataset analysis of high-throughput omics data often leads to unsatisfactory results. The integrative analysis of heterogeneous raw data from multiple independent studies provides an effective way to increase sample size and improve marker selection results. In integrative analysis, the regression coefficient matrix has certain structures. In our study, we use group penalization for one- or two-dimensional marker selection and introduce contrast penalties to accommodate the subtle coefficient structures. Simulations show that the proposed methods have significantly improved marker selection properties. In the analysis of cancer genomic data, important markers missed by the existing methods are identified.

A Computationally Fast and Asymptotically Efficient Estimating Approach for Change-points

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Abstract. The existence of one or more change-points in linear regression problems has significant applications in climate data, economic time series and for modeling biological processes, where the change-points mostly pertain to the onset of biologically important phenomena. Estimation of change-point(s) in a broken-stick model using the exact likelihood has been discussed in some depth in the literature, but most of the methods are computationally quite expensive: the non-differentiability at the kink(s) necessitates an exhaustive search across tuples of order statistics. In this talk, I will present a local smoothing approach to address this difficulty, where the broken-stick is smoothed in a shrinking neighborhood of the kinks by quadratic functions. This is used as our working model, which allows the use of Newton-Raphson type methods for the working likelihood function. We find that the estimates converge at root-n rate and are asymptotically normal and fully efficient. Simulations clearly vindicate the computational economy of the approach with quite remarkable gains in computation times for the two change-points problem. We implement our method on a data set from a crop research experiment.

This is a joint work with Ritabrata Das and Moulinath Banerjee.

Personalized Treatment for Longitudinal Data

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Abstract. We develop new modeling and estimation for personalized treatment for individuals with high heterogeneity. Incorporating subject-specific information into treatment subgroup is critical since individuals could react to the same treatment quite differently. We propose to identify subgroups with longitudinal observations through random-effects estimation where the random effects are not necessarily normal distributed. The advantage of this approach is that we can quantify intrinsic associations between unobserved subject-specific effects and observed treatment outcomes, and therefore provide optimal treatment assignments for different individuals. In contrast, traditional mixed-effects models assuming normal distribution cannot effectively distinguish different patterns of treatment effects. We develop asymptotic consistency theory for individual treatment effect estimation, and show that the new estimator is more efficient than the random effect estimator which ignores correlation information from longitudinal data. Simulation studies and a data example from an AIDS clinical trial group confirm that the proposed method is quite efficient in identifying an effective treatment strategy for subgroups in finite samples.

This is joint work with Hyunkeun Cho and Peng Wang.

Analysis of Merged Longitudinal Data from Multiple Studies

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Abstract. When merging subject-level data from multiple longitudinal studies is undertaken, different strategies of processing information may be considered to build up statistical estimation and inference. It is possible to combine study-specific estimates, or to join study-specific estimating functions, or to integrate data sets. The currently popular strategy of meta analysis is to directly combine estimates, and a retreat of this approach will be given in the talk. As an alternative, a new approach to combining estimating functions is proposed and compared in detail with some existing methods. Examples will be used to illustrate the comparison of individual strategies of data merging.

Hidden Markov Latent Variable Models with Multivariate Longitudinal Data

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Abstract. This paper develops a hidden Markov latent variable model for analyzing multivariate longitudinal data. The latent variable model is defined in a structural equation modeling framework, in which a measurement equation measures latent constructs through multiple longitudinal responses, and a structural equation examines the interrelationships among observed and latent variables. To reveal the dynamic patterns and possible heterogeneity of the above mentioned associations and interrelationships, a mixed hidden Markov model is introduced to model the transition probabilities across different latent states. We develop a maximum likelihood procedure to analyze the proposed model. The asymptotic properties of the parameter estimates, and theWald- and Score-type statistics for testing the heterogeneity of model parameters are established. The Monte Carlo expectation conditional maximization algorithm is employed to obtain the estimates of unknown parameters. The Gibbs sampler coupled with the forward-backward recursion sampling is implemented in the Monte Carlo expectation-step. We conduct simulation studies to assess the performance of the proposed methodologies and apply the model to a longitudinal study of cocaine use.

Modeling and Estimating the Terminal Behavior of a Recurrent Marker Process

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Abstract. Recurrent events and marker processes often exhibit meaningful terminal behavior during a time period before the failure event. A natural and direct way to study such terminal behavior is to align the processes using failure events as time origins. This talk discusses estimation and regression modeling of a recurrent marker process by counting time backward from the failure event. A three-level semiparametric regression model is proposed for jointly modeling time to failure event, backward recurrent event process, and markers associated with recurrent events. The first level is a proportional hazards model for failure time, the second level is a proportional rate model for recurrent event processes before death and the third level is a proportional mean model for markers given a recurrent event occurrence before death. Estimating equations for marked counting processes are proposed to estimate the regression parameters in the three-level regression models. The proposed methods are illustrated by real data examples.

This is joint work with Kwun Chuen Gary Chan.

Sieve Maximum Likelihood Estimation for a General Class of Accelerated Hazards Models

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Abstract. In semiparametric hazard regression, nonparametric components may involve unknown regression parameters. Such intertwining effects make model estimation and inference much more difficult than the case in which the parametric and nonparametric components can be separated out. We study the sieve maximum likelihood estimation for a general class of hazard regression models, which include the proportional hazards model, the accelerated failure time model, and the accelerated hazards model. Coupled with the cubic B-spline, we propose semiparametric efficient estimators for the parameters that are bundled inside the nonparametric component. We overcome the challenges due to intertwining effects of the bundled parameters, and establish the consistency and asymptotic normality properties of the estimators. We carry out simulation studies to examine the finite-sample properties of the proposed method, and demonstrate its efficiency gain over the conventional estimating equation approach. For illustration, we apply our proposed method to a study of bone marrow transplantation for patients with acute leukemia.

Joint with Dr. Xingqiu Zhao and Dr. Guosheng Yin

Estimation and Selection via Lasso and Its Multistage Adaptive Applications

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Abstract. The ℓ_1-penalized method, or the Lasso, has emerged as an important tool for the analysis of large data sets. Many important results have been obtained for the Lasso in linear regression which have led to a deeper understanding of high-dimensional statistical problems. We consider a class of weighted ℓ_1-penalized estimators for convex loss functions of a general form, including the generalized linear models. We study the estimation, prediction, selection and sparsity properties of the weighted ℓ_1-penalized estimator in sparse, high-dimensional settings where the number of predictors p can be much larger than the sample size n. Adaptive Lasso is considered as a special case. A multistage method is developed to approximate concave regularized estimation by applying an adaptive Lasso recursively. We provide prediction and estimation oracle inequalities for single- and multi-stage estimators, a general selection consistency theorem, and an upper bound for the dimension of the Lasso estimator. Important models including the linear regression, logistic regression and log- linear models are used throughout to illustrate the applications of the general results.

This is based on joint work with Jian Huang.

Contributed Talks

On Analysis of Warranty Data with Unobserved Sales Date

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Abstract Most commercial products in the market place are sold with warranties and they are sold indirectly through dealers. This results in serious missing data problems in the analysis of field return data because of the unobserved sales date for the unreturned units. Our purpose here is to systematically investigate the parametric and nonparametric inference for such data. In particular, we are interested in the distributions of the sales lag, which is only observed for the returned units and can be regarded as the customer demand rate when exponential distribution is imposed, and the lifetime (time from purchase to failure) of the product under study. Estimation of the sales lag is important for production and inventory scheduling while the lifetime distribution reflects failures under real use conditions. We first discuss the parametric estimation where a joint parametric distribution is imposed on the sales lag and the lifetime. A stochastic expectation-maximization (SEM) framework is proposed for the inference. Next, we consider nonparametric estimation with the help of spline functions. An SEM procedure is devised for the spline-based inference and investigation of the asymptotic properties of the sieve estimators is under way.

Real-time spatial forecasting system for multiple air pollutants

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Abstract Accurate, instantaneous and high resolution spatial air pollution information can better inform the general public and policy makers of the air pollution levels that could cause adverse health effects. This talk focuses on an example of a spatio-temporal models for forecasting ground level ozone concentration levels over a vast study region in the eastern United States. These models incorporate output from a computer simulation model known as the Community Multi-scale Air Quality (Eta-CMAQ) forecast simulation model under the hierarchical Bayesian modeling framework. An introduction to the onging project on Hong Kong multiple air pollutants real-time forecasts will be given as a further example.

Stream 4
Mathematical Modeling and Computational Mathematics

Invited Talks

Error Estimates and Superconvergence of Mixed Finite Element Methods for Bilinear Optimal Control Problems

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Abstract. With the advances of scientific computing, optimal control problems are now widely used in multi-disciplinary applications such as physical, biological, medicine, engineering design, finance, fluid mechanics, and social-economic systems etc. As a result, more and more people will benefit greatly by learning to solve the optimal control problems numerically. Realizing such growing needs, books and papers on optimal control put more weight on numerical methods. There has been very extensive studies in a priori/posteriori error estimates and superconvergence analysis of finite element methods for optimal control problems governed by elliptic or time dependent equations (parabolic equations, hyperbolic equations, Navier-Stokes equations) etc.

Bilinear optimal control problem is of course a class of optimal control problem. In engineering design work, there exist widely bilinear optimal control problems. For example, parameter estimation problems, optimal shape design, Stokes flow matching problems, electrochemical machining design problems, optimal design of stationary flow. In comparison with the standard optimal control problems, there were relatively fewer known results in finite element approximation for bilinear optimal control problem due to the lower regularity of the control variable. Due to the lower regularity, it is more difficult to obtain error estimates for bilinear optimal control problems include a useful model problem of parameter estimation.

In this work, we investigate error estimates and superconvergence of the bilinear elliptic optimal control problems by Raviart-Thomas mixed finite element methods. The control variable enters the state equation as a coefficient. The state and the co-state variables are approximated by Raviart-Thomas mixed finite element spaces and the control variable is approximated by piecewise linear or constant functions. We obtain the superconvergence property between average L^2 projection and the approximation of the control variable, the convergence order is h^2. Finally, we derive a prioti and a posteriori error estimates for the control variable and coupled state variable.

Minimal Residual Methods for Solving Singular Unsymmetric or Non-Hermitian Linear Equations

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Abstract. GMRES (Saad and Schultz 1986) is a famed minimal-residual method for solving nonsingular unsymmetric or non-Hermitian linear systems. It may suffer non-benign breakdown on nearly singular systems (Brown and Walker 1997). When working, the solver returns only a least-squares solution for a singular problem (Reichel and Ye 2005).

We present GMRES-QLP, a successful revamp of GMRES, for returning the unique pseudoinverse solutions of singular or ill-conditioned linear systems or linear least-squares problems. On nonsingular problems, it is numerically more stable than GMRES. In any case, users do not need to know a priori whether the systems are singular, ill-conditioned, or compatible; the solver constructively reveal such properties. It leverages the QLP decomposition (Stewart 1999) to reveal the rank of the Hessenberg matrix from the Arnoldi process, incurring only minor additional computational cost in comparison to GMRES. We present extensive numerical experiments to demonstrate the scalability and robustness of the solver, with or without preconditioners or restart.

This is ongoing work by the speaker.

Nonlocal Calculus, Nonlocal Balance Laws and Asymptotically Compatible Discretizations

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Abstract. Nonlocality is ubiquitous in nature. While partial differential equations (PDE) have been used as effective models of many physical processes, nonlocal models and nonlocal balanced laws are also attracting more and more attentions as possible alternatives to treat anomalous process and singular behavior. In this talk, we exploit the use of a recently developed nonlocal vector calculus to study a class of constrained value problems on bounded domains associated with some nonlocal balance laws. The nonlocal calculus of variations then offers striking analogies between nonlocal model and classical local PDE models as well as the notion of local and nonlocal fluxes. We discuss the consistency of nonlocal models to local PDE limits as the horizon, which measures the range of nonlocal interactions, approaches zero. In addition, we present asymptotically compatible discretizations that provide convergent approximations in the nonlocal setting with a nonzero horizon and are also convergent asymptotically to the local limit as both the horizon and the mesh size are taking to zero. Such asymptotically compatible discretizations can be more robust for multiscale problems with varying length scales.

An Efficient Numerical Approach for High Frequency Wave Scattering in Random Media

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Wave scattering in random media arises in many scientific and engineering fields including geoscience, image science, materials science and medical science. Computing quantities of interest for the solutions of such wave problems, especially, in the high frequency case, poses a daunting computational challenge because of sheer amount of computations required to solve those problems. Due to their strong indefiniteness, highly oscillatory nature of solutions, and lack of efficient iterative solvers, standard numerical approaches such as brute force Monte Carlo method, sparse grid method, and polynomial chaos method are either too expensive to use or do not work well. In this talk I shall present a newly developed multi-resolution approach for the random Helmholtz problem with large wave numbers. In this approach the original random Helmholtz problem is reduced to a finite number of deterministic and non-homogeneous Helmholtz problems with random source terms, which are discretized by some unconditionally stable discontinuous Galerkin methods. An efficient solver with computational complexity of order $O(3N^3/2)$ is also proposed to solve the resulting algebraic problems. Convergence analysis and numerical experiments will be presented to demonstrate the potential advantages of the proposed numerical approach. Extensions to random elastic and electromagnetic wave equations will also be discussed.

The material of this talk is based on a joint work with Cody Lorton of the University of Tennessee, U.S.A. and Junshan Lin of Auburn University, U.S.A.

Phase-Field Modeling, Isogeometric Analysis and Unconditionally Stable Time Integration: Application to Biological Interfaces

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Abstract. There are many processes in engineering and natural sciences that involve the evolution of interfaces. Prime examples include interfaces between several distinct states arising in mixtures and multiphase systems such as two-phase flows, binary alloys, fluid phase transition, grain growth, and even the growth of cancerous tumors. Phase-field modeling refers to a particular mathematical description of a system with evolving interfaces. The key idea is that interfaces are described by a smoothly changing phase field. The phase field is governed by a partial differential equation, which tracks the so-called *diffuse interfaces* and encodes the interfacial physics at once. The systems are inherently nonlinear equations with higher-order spatial derivatives that account for the interfacial forces. Moreover, the higher-order terms are

scaled with a small coefficient that makes the equations singularly perturbed. Phase-field models, thus, bring a new set of challenges for numerical simulations, such as, for example, stiff semi-discretizations, stable time-stepping algorithms and the treatment of sharp internal layers.

The higher-order partial-differential operators typically present in phase-field equations are difficult to deal with by standard finite element approaches that utilize C^0 trial and weighting functions. Our approach is based on Isogeometric Analysis, permitting simple and efficient discretizations through the use of continuously differentiable splines. I will present results for the Cahn-Hilliard equation, a two-phase model applicable to the segregation of phases in binary alloys. We have also applied our methodology to the Navier-Stokes-Korteweg equations, which describe water/water-vapor two-phase flow. I will present solutions involving condensing vapor bubbles in two and three dimensions.

Finally, I will present our new unconditionally stable method for the phase-field equations. Our algorithm is second-order accurate and inherits the nonlinear stability properties of the continuum theories.

I will finalize by presenting the application of the above ideas to the problem of capillary growth in tumor angiogenesis.

Fundamental Convergence Theorems of Numerical Methods for SDEs

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Abstract. In this talk we review theoretical results on the mean-square convergence of numerical methods for stochastic ordinary differential equations, stochastic delay differential equations, neutral stochastic delay differential equations, jump-diffusion differential equations, neutral stochastic delay differential equations with jump-diffusion, stochastic partial differential equations and backward stochastic differential equations. These results are called fundamental convergence theorems of numerical methods for stochastic differential equations.

An Adaptive Time Stepping Method with Efficient Error Control for Second-Order Evolution Problems

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Abstract. This talk is concerned with time stepping finite element methods for abstract second order evolution problems. We will derive optimal order a posteriori error estimates and a posteriori nodal superconvergence error estimates using the energy approach and the duality argument. With the help of the a posteriori error estimator developed in this work, we will further propose an adaptive time stepping strategy. A number of numerical experiments are

performed to illustrate the reliability and efficiency of the a posteriori error estimates and to assess the effectiveness of the proposed adaptive time stepping method.

This is a joint work with Junjiang Lai and Tao Tang.

Fluid-Structure Interaction Model and Levelset Method

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Abstract. We derive a weak form and weak solution of the level set formulation of Cottet and Maitre for fluid-structure interaction problems with immersed surfaces. The method in particular exhibits appealing mass and energy conservation properties and provides a variational formulation of Peskin's Immersed Boundary methods.

Fast Explicit Integration Factor Methods for Semilinear Parabolic Equations

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Abstract. In this talk, we present a numerical method and its fast implementation for the solution of a wide class of semilinear parabolic equations including the Allen-Cahn equation as a special case. The method combines efficient decompositions of spatial difference operators on a regular mesh with stable and accurate exponential time integrators. It can deal with stiff nonlinearity and both homogeneous and inhomogeneous boundary conditions of different types. Numerical experiments demonstrate effectiveness of the new approach for both linear and nonlinear model problems.

Partial Differential Equations Using Reduced-Order Modeling

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Abstract. Computing approximations of solutions of Navier-Stokes equations is a computationally intensive task. For realistic simulations, many thousands or even millions of degrees of freedom are often required to obtain useful approximations. Thus, if one needs to do multiple simulations or to do a simulation in real time, the use of reduced-order modeling (ROM) should be considered.

For approximating the solution $u(t,x)$ of a nonlinear, time dependent PDEs, the type of ROMs proceed as follows.

(1) One collects samples of solutions of the nonlinear PDE to produce a set of snapshot sets.
(2) One choose a reduced basis $\{\phi_i(x)\}_i^d = 1$; hopefuly, d is very small compare to the usual number of functions used in a high fidelity problem.
(3) One seeks an approximation $u_{rom}(t,x)$ to the state u of the form

$$u_{rom}(t,x) = \sum_{j=1}^{d} a_j(t)\phi_j(x).$$

(4) Then, one determine the coefficients $a_j, j = 1, \dots, d$, by solving the state equations in low-dimensional space.

We consider the CVT and POD approach. We focus on how to generate snapshots which hopefully will accurately represent the dynamical behavior of those solutions. Then, we will study on how to determine ROM basis using snapshots which one again hopes, can accurately capture the information contained in the snapshot set. We also investigate optimal control problems for Navier-Stokes flows. A discussion of reduced-order modeling for Navier-Stokes flow is given to provide a context for the construction and application of reduced-order bases. Reviews of the POD (proper orthogonal decomposition) and CVT (centroidal Voronoi tessellation) approaches to reduced-order modeling are provided, including descriptions of POD and CVT reduced-order bases, their construction from snapshot sets, and their application to the ROM based optimal control problems for the Navier-Stokes system.

Augmented IFEM for Interface and Irregular Domain Problems

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Abstract. Augmented immersed finite element methods (AIFEM) are proposed to solve elliptic interface problems with piecewise discontinuous coefficients and non-homogeneous jump conditions; and Poisson equations on irregular domains. Based on the framework of the immersed finite element method (IFEM), a uniform triangulation is used so that a fast Poisson solver can be used. The non-homogeneous jump conditions in the solution and the flux are treated as source terms using the source removal technique. For the piecewise constant but discontinuous coefficient case, we transform the original elliptic interface problem to a Poisson equation with the same jump in the solution, but a unknown flux jump (an augmented variable) which is chosen such that the original flux jump condition is satisfied.

In discretization, the GMRES iteration is used to solve the augmented variable which has co-dimension one compared with that of the solution. The core of each GMRES iteration involves solving a Poisson equation using a fast Poisson solver and an interpolation scheme to interpolate the flux jump condition. Numerical experiments showed that the number of the GMRES iteration is independent of the mesh size and the jump in the coefficient. Not only, the computed solution is second order accurate in the L^∞ norm using the developed method, the

computed normal derivative is also second order accurate. The AIFEM developed for interface problems has also been extended to Poisson equations on irregular domains with some slight modifications.

This is a joint work with Haifeng Ji and Jinru Chen.

A Conservative Scheme for Poisson-Nernst-Planck Equations

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Abstract. A macroscopic model to describe the dynamics of ion transport in ion channels is the Poisson-Nernst-Planck (PNP) equations. In this talk, we will present a finite-difference method for solving PNP equations, which is second-order accurate in both space and time. We use the physical parameters specifically suited toward the modeling of ion channels. We introduce a simple iterative scheme to solve the system of nonlinear equations resulting from discretizing the equations implicitly in time, which converges in a few iterations. We place emphasis on ensuring numerical methods to have the same physical properties that the PNP equations themselves also possess, namely conservation of total ions and correct rates of energy dissipation. Further, we illustrate that, using realistic values of the physical parameters, the conservation property is critical in obtaining correct numerical solutions over long time scales.

Energy Law and Its Numerical Preservation for Quasi-Incompressible Navier-Stokes Cahn-Hilliard (NSCH) System with Variable Density

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Abstract. We will present some recent work on a phase-field model for multiphase fluids with variable densities. A Quasi-Incompressible NSCH System for the model will be investigated. Under a minor reformulation of the system we show that there is a continuous energy law underlying the system, assuming that all variables have reasonable regularities. For the reformulated system we then design a C^0 finite element method and a special temporal scheme where the energy law is preserved at the discrete level. Such a discrete energy law (almost the same as the continuous energy law) for a variable density two-phase flow model has never been established before with C^0 finite element. Some numerical results will be presented to demonstrate the capabilities of our numerical schemes. We will also show an example that an energy law preserving method will perform better for multiphase flow problems.

Efficient Energy Stable Schemes for Phase-Field Models of Two-Phase-Flows with Variable Density

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Abstract. I shall present some recent work on phase-field models for two-phase flows with variable density. We shall consider phase-field models which enforce either the incompressibility or mass conservation within the interfacial region, and construct efficient (in some cases totally decoupled) energy stable schemes.

Four Color Theorem and Convex Relaxation for Image Segmentation with Any Number of Regions

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Abstract. Image segmentation is an essential problem in imaging science. One of the most successful segmentation models is the piecewise constant Mumford-Shah minimization model. This minimization problem is however difficult to carry out, mainly due to the non-convexity of the energy. Recent advances based on convex relaxation methods allow to estimate almost perfectly the geometry of the regions to be segmented when the mean intensity and the number of segmented regions are known a priori. The next important challenge is to provide a tight approximation of the optimal geometry, mean intensity and the number of regions simultaneously while keeping the computational time and memory usage reasonable. In this work, we propose a new algorithm that combines convex relaxation methods with the four color theorem to deal with the unsupervised segmentation problem. More precisely, the proposed algorithm can segment any a priori unknown number of regions with only four intensity functions and four indicator ("labeling") functions. The number of regions in our segmentation model is decided by one parameter that controls the regularization strength of the geometry, i.e. the total length of the boundary of all the regions. The segmented image function can take as many constant values as are needed.

This talk is based on jont works with T. F. Chan, X. Bresson and R. Zhang.

Numerical Stability on the Allen-Cahn Equation

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Abstract. The AllenCahn equation is a reaction-diffusion equation of mathematical physics which describes the process of phase separation. In this talk, we will discuss a new framework on establishing the numerical stability in the maximum norm for the Allen-Cahn equation. Extension to Allen-Cahn equation with fractional-in-space will be discussed also.

Numerical Schemes for the Modified Phase Field Crystal (MPFC) Equation with Unconditional Pseudo-Energy Stability

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Abstract. Both the first and second order accurate convexity splitting schemes for the Modified Phase Field Crystal (MPFC) equation, a generalized damped wave equation for which the usual Phase Field Crystal (PFC) equation is a special degenerate case, are presented in the talk. Both schemes are proven to be unconditionally pseudo-energy stable. Numerical results are presented to demonstrate the accuracy, energy stability and the efficiency of the schemes. The relaxation properties of the MPFC model, compared with the standard PFC model, are observed in the numerical simulation.

Numerical schemes for long time statistical properties of dissipative chaotic dynamical systems

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Abstract. Many important systems such as those that govern the motion of the atmosphere and oceans are chaotic. It is well-known that statistical properties are much more important and relevant than a single trajectory for such kind of systems. One of the practical challenges is the design of accurate and efficient numerical schemes that are able to capture the long time statistical properties or the climate of the underlying system. In this talk, we will discuss methodologies that can be used to design numerical schemes that are able to capture long time statistical properties of chaotic dynamical systems governed by dissipative partial differential equations. In particular, we will present criteria in terms of temporal, spatial, and fully discretized algorithms that guarantee the desired convergence of long time statistical properties. Noise effect will be discussed as well.

New Nonlocal Continuum Electrostatic Models and Fast Finite Element Solvers for Biomolecule in Ionic Solvent

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Abstract. Calculation of electrostatic potential energy for biomolecule (such as protein and DNA) in ionic solvent is a fundamental task in the study of biomolecular structure, catalytic activity, and ligand association. To reflect the polarization correlations among water molecules, nonlocal dielectric models were developed in the last thirty years, and were recognized to be more accurate than their corresponding local dielectric models in the calculation of electrostatics. However, they were expensive to be solved numerically, and only limited to pure water solvent due to modeling and algorithmic complications. None of them incorporate any ionic solvent.

To change this situation, we recently developed new nonlocal dielectric models, fast finite element solvers, and computer program packages for biomolecule in both pure water and ionic solvent. In this talk, I will give them a short review. I then will report a new nonlocal Poisson-Boltzmann Equation (PBE) model, and a new analysis on the solution existence and uniqueness for local and nonlocal PBE models. Furthermore, I will present a new solution decomposition scheme for solving local and nonlocal PBE models. Finally, numerical tests on proteins and a Born ball model with an analytical solution are reported, which validate the new solution decomposition scheme and demonstrate the efficiency of our finite element program package.
This work is supported in part by NSF grant #DMS-1226259 and the UWM Research Growth Initiative.

Some New Developments of Spectral and Spectral Element Methods and Their Applications

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Abstract. In this talk, we present some new developments in spectral (element) methods for some fractional integral/differential equations. The main ingredients include:

(1) Parareal methods for integral equations;
(2) High order methods for abnormal diffusion equations;
(3) Spectral (element) methods for fractional partial differential equations.

We will explain a number of fractional models using the stochastic formulation of transport phenomena in terms of a random walk process, and present some efficient methods for the numerical solution of the time-space fractional diffusion equation. Some interesting applications to viscoelastic materials, turbulence, and molecular biology will be addressed.

The Phase Transition and Large Deformation Theory of Macromolecular Microsphere Composite Hydrogel

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Abstract. In this talk, I will present the phase transition process and large deformation theory of Macromolecular Microsphere Composite (MMC) Hydrogel.

Firstly, we use the Time-Dependent Ginzburg-Landau (TDGL) mesoscopic model to simulate the phase transition process of macromolecule microsphere composite (MMC) hydrogel. We propose a free energy for such a reticular structure according to the structures of MMC hydrogel and entropy theory. This work generalizes the mean field theory confined by Flory-Huggins for free energy in a polymer blend system. A spectral method is adopted to numerically solve the MMC-TDGL equation. The numerical results are consistent with chemical experiments, showing the network structure. According to the numerical results at different temperatures, we understand that the system shows intermittent phenomenon with increasing reaction temperature, which is a very good explanation of chemical experiments.

Then we investigate the large deformation theory for the macromolecular microsphere composite hydrogel. It is presented the the large deformation model. Simulation result are completely consistent with the chemical experiment for the strain-stress relation. So this theory can be extended other soft matters.

The Small Deborah Number Limit of the Doi-Onsager Equation to the Ericksen-Leslie Equation

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Abstract. We present a rigorous derivation of the Ericksen-Leslie equation starting from the Doi-Onsager equation. As in the fluid dynamic limit of the Boltzmann equation, we first make the Hilbert expansion for the solution of the Doi-Onsager equation. The existence of the Hilbert expansion is connected to an open question whether the energy of the Ericksen-Leslie equation is dissipated. We show that the energy is dissipated for the Ericksen-Leslie equation derived from the Doi-Onsager equation. The most difficult step is to prove a uniform bound for the remainder in the Hilbert expansion. This question is connected to the spectral stability of the linearized Doi-Onsager operator around a critical point. By introducing two important auxiliary operators, the detailed spectral information is obtained for the linearized operator around all critical points. However, these are not enough to justify the small Deborah number limit for the inhomogeneous Doi-Onsager equation, since the elastic stress in the velocity equation is also strongly singular. For this, we need to establish a precise lower bound for a bilinear form associated with the linearized operator. In the bilinear form, the interactions between the part inside the kernel and the part outside the kernel of the linearized operator are very complicated. We find a coordinate

transform and introduce a five dimensional space called the Maier-Saupe space such that the interactions between two parts can been seen explicitly by a delicate argument of completing the square. However, the lower bound is very weak for the part inside the Maier-Saupe space. In order to apply them to the error estimates, we have to analyze the structure of the singular terms and introduce a suitable energy functional.

Furthermore, we prove the local well-posedness of the Ericksen-Leslie system, and the global well-posednss for small initial data under the physical constrain condition on the Leslie coefficients, which ensures that the energy of the system is dissipated. Instead of the Ginzburg-Landau approximation, we construct an approximate system with the dissipated energy based on a new formulation of the system.

Contributed Talks

A New Modified Adomian Decomposition Method for Solving Robin Boundary Value Problems for Second-Order Differential Equations

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Abstract. The purpose of this paper is to investigate the application of the Adomian decomposition method (ADM) for solving boundary value problems for second-order differential equations with Robin boundary conditions. We first reformulate the boundary value problems for linear equations as a fixed point problems for a linear Fredholm integral operator, and then apply the ADM. We also extend our approach to include second-order nonlinear differential equations subject Robin boundary conditions.

A Sub-cell real 2D WENO Reconstruction Method for Spatial Derivatives in the ADER Scheme

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Abstract. We introduce a real 2D sub-cell WENO reconstruction method to evaluate spatial derivatives in the 5th-order ADER scheme. For the 5th-order ADER scheme in two dimensions, the basic idea in our reconstruction is to use only 3×3 stencils to reconstruct 14 point-wise values of solutions which are used to reconstruct the distribution function of solutions used to evaluate all spatial derivatives with high-order accuracy. In the original ADER scheme of Titarev and Toro (1) , the dimension-by-dimension directly reconstructed method is used and 5×5 stencils are used to reconstruct polynomials for solutions and spatial derivatives in two dimension. In the 5th-order sub-cell ADER scheme of Cheng et al (2), the dimension-by-dimension sub-cell reconstruction approach for spatial derivatives is employed in two dimension and 25 point-wise values of solutions are evaluated which are used to obtain the spatial derivatives. Comparing the other two reconstruction method, the real 2D sub-cell WENO reconstruction method not only reduces greatly the computational costs of the ADER scheme on a given mesh, but also avoids possible numerical oscillations near discontinuities, as demonstrated by a number of two-dimensional numerical tests. All these tests show that the 5th-order ADER scheme based on our real 2D sub-cell reconstruction method achieves the desired accuracy, and is essentially non-oscillatory and computationally cheaper for problems with discontinuities.

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Effects of a Static Bottleneck in a Continuum Traffic Flow Model

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We have investigated the effects of a static bottleneck on traffic flow using a continuum speed-gradient model with open boundary conditions. The location of bottleneck is assumed to be in the middle of the road. It has been found that the static bottleneck affects the uniform traffic flow significantly. The spatio-temporal evolution of density shows that the traffic exists in distinct states and the phase transitions from one state to another have been discussed. We have also developed the phase diagram with respect to different initial homogenous densities. Additionally, the effect of strength of bottleneck on the phases has also been examined.

A Study on Influence of Changing Poling Direction on Piezoelectric Plate Cut along Two Unequal Cracks

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Abstract. It is well-known that a wide range of poled piezoelectric ceramics retains their aligned electric dipole field in the material microstructure below Curie temperature. This electric poling direction affects the material properties and fracture behavior. Numerous studies have demonstrate that crack orientation as well as electric poling direction greatly influences crack growth. Simultaneously impermeable, permeable and semi-permeable conditions on the crack faces also affects the behavior of piezoelectric ceramic. It is noted that impermeable and permeable conditions, respectively, give higher and lower estimate of energy release rate etc. But empirically it is observed that semi-permeable boundary condition give more accurate results.

The effect of change in poling direction for the case of single crack has been reported in literature. But the case of multiple cracks under changing poling direction is yet not addressed. The aim of this paper is to address this paucity. In the present work, a poled piezoelectric medium cut along two unequal collinear straight cracks. The cracks are assumed to be traction free and inside cracks gaps the semi-permeable boundary condition prevail. Combine in-plane uniform

constant normal(to the faces of cracks) mechanical and electrical-displacement are prescribed at remote boundary of the plate. The mathematical model obtained using Stroh formalism and is solved using complex variable technique. Closed form expressions are derived for crack opening displacement (COD), crack opening potential drop (COP), intensity factors (IFs) and energy release rate (ERR).

A case study is presented for poled PZT-5H ceramic using proposed model. The effect of change in poling direction is plotted for IFs and ERR. It is observed that as poling direction is moved from the crack length axis to the normal of crack length IFs and ERR continuously increases linearly and attain their maximum values when poling direction is perpendicular to the crack length.

Numerical Solutions of One and Two Dimensional Integral Equations

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Abstract. Integral equations are useful in many branches of mathematics and science as well. We begin with a survey of various methods in solving different kinds of integral equations, namely, Fredholm Integral equation of the first and the second kind, Volterra integral equation of the second kind and Fredholm-Volterra integral equation as well as the discussions of singular and nonlinear integral equations. We will also discuss solving two-dimensional integral equations. There are many different methods of solving integral equations. Wavelet based methods are of particular interest. The localization property, robustness and other features of wavelets are essential to solving integral equations efficiently. We will present a wavelet based method together with several convergence results of the method. A few examples will also be presented. As a consequence of these examples, we will compare the results with other methods.

Mathematically Modeling Patent Precedents and Inventions Disclosed by Patents, —First Steps of a “Mathematical Theory of Innovation”

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Abstract. Any innovation alias invention embodies technically creative steps not limited to dealing with tangible subject matter, but comprising any allegedly new technique teaching $TT.0$ disclosed in an enabling way by a document, often a patent, $TT.0$ being non-obvious over pertinent ordinary skill(s) and prior art. The latter is represented by a reference set of additional documents, each disclosing a $TT.i$, $1 \leq i \leq I$, which jointly potentially anticipate $TT.0$. The paper provides the mathematical tools for modeling the innovation/invention/$TT.0$

embodied by e.g. a patent over its prior art and outlines actually modeling it by them and determining its creative and pragmatic heights over a given reference set. These axiomatically defined mathematical tools are founded by/on several important Highest Courts' patent precedents. They enable providing the first mathematical analysis of their 2012 spectacular patenting decisions, e.g. *MAYO clinic vs. PROMETHEUS labs* on drugs or *ASS. FOR MOLECULAR PATHOLOGY vs. MYRIAD labs* on human genomes.

Due to the unquestionable foundation of this mathematical modeling of the fundamental patent problems involved - as to patentability of such inventions in the US under 35 USC §§ 101, 102/103, 112, and in Europe not yet discussed - this approach to patent jurisdiction is expected to soon become called "patent technology". But this scientific approach to mathematically modeling and analyzing the quality and quantity of the innovativity/creativity actually embodied by an alleged invention/innovation reaches much further beyond the area of patenting. It hence is supposed to provide the first - but already really substantial - steps to a "Mathematical Theory of Innovation", currently powerfully evolving as a mathematically unusually rigorous "Patent Technology".

Strip-Saturation Model for Piezoelectric Strip Cut along Two Collinear Cracks under Mode-III Deformation

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Abstract. The problem of an infinitely long transversely isotropic piezoelectric strip weakened by two equal lengths collinear cracks is addressed. The strip is assumed to be poled electrically perpendicular to the crack surface. Two quasi- static collinear cracks are situated transversely in the strip and symmetrically oriented with respect to the middle line of the strip. Crack rims are free of mechanical load and electric charge. Combined anti-plane shear stress and in-plane electric-displacement prescribed at the remote boundaries of the strip. Consequently, the strip yields both mechanically and electrically. Hence electric strip-zones protrudes ahead each tip of the cracks. The piezoelectric ceramic being mechanically brittle, the developed mechanical zone is assumed to be of negligible small. The developed strip-electric zones are prescribed in-plane normal cohesive polarization limit electric-displacement. The cracks are arrested from further opening.

The analytical solution of the mathematical model framed of the problem solved using Fourier series method. Which reduces the problem to solution of two sets of triple series equation with cosine kernel. Each of triple series equation is further reduced to singular integral equations with Cauchy kernel of first kind, which in turn is solved numerically.

Closed form analytic expressions are derived at both inner and outer crack tips to calculate saturation zone length, crack sliding displacement (CSD), crack opening potential drop (COP), stress intensity factor (SIF), electric displacement intensity factor (EDIF) and energy release rate (ERR).

Numerical illustrative case study is presented to show the effect of applied loading on fracture

parameters viz. SIF, EDIF, EER, COP, CSD etc. at inner and outer crack tips for poled PZT-4 piezoelectric ceramic. The results confirm the model is capable of crack arrest under small-scale yielding.

A Multilevel Correction Method for Transmission Eigenvalue Problems

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Abstract. In this lecture, we will introduce a type of multilevel correction method for eigenvalue problems. In this type of correction method, we can do the correction steps by any times which can improve the overall efficiency for solving eigenvalue problems. Based on the multilevel correction method, we construct a multigrid method to solve the transmission eigenvalue problem with optimal computational complexity.

An Energy-stable Finite-Difference Scheme for the Binary Fluid-Surfacant System

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Abstract. We present an unconditionally energy stable finite-difference scheme for the binary fluid-surfactant system. The proposed method is based on the convex splitting of the energy functional with two variables. Here are two distinct features: (i) the convex splitting energy method is applied to energy functional with two variables, and (ii) the stability issue is related to the decay of the corresponding energy. The full discrete scheme leads to a decoupled system including a linear sub-system and a nonlinear sub-system. Algebraic multigrid and Newton-multigrid methods are adopted to solve the linear and nonlinear systems, respectively. Numerical experiments are shown to verify the stability of such a scheme. The present numerical results are in good agreement with the existing ones.

Stream 5

Numerical Multi-Linear Algebra and Tensor Computation

Invited Talks

Z-Eigenvalues of the Adjacency Tensors for Uniform Hypergraphs

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Abstract. The adjacency matrices for graphs have been generalized to the adjacency tensors for uniform hypergraphs by J.Cooper in 2012. In this talk, we present some fundamental properties for the adjacency tensor and its Z-eigenvalues of a uniform hypergraph. Bounds on the smallest and the largest Z-eigenvalues of the adjacency tensors for uniform hypergraphs are obtained. Moreover, some inequalities between these two Z-eigenvalues and other hypergraph parameters have been created.

Tensor Networks and Multilinear Low-rank Approximations for Big Data Analysis

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Abstract. Tensor decompositions (TD) and tensor networks (TN) are promising tools for data analytics and mining. Despite exist many efficient and powerful algorithms for TD and TN, scalability to large datasets for such decomposition algorithms is still a challenging problem. In this talk we review basic and emerging new models and associated learning algorithms for large-scale tensor networks and tensor decompositions including, PARAFAC/CANDECOMP (CPD), Tensor Train, (TT), Hierarchical Tucker (HT) decompositions, HOSVD, and Hierarchical Outer Product Decomposition (HOPT). We will discus a problem of tensorization (i.e., creating very high-order tensors from lower-dimensional original data (vectors, matrices and/or low-order tensors) and super compression of data via quantized tensor networks. The purpose of a tensorization or reshaping is to achieve via low rank tensor decompositions "super" compression and meaningful compact representation of structured data. We also discuss how to overcome the curse of dimensionality via tensor networks and divide-and-conquer approaches.

This is joint work with Dr. Guoxu Zhou.

Compressive Sensing of Sparse Tensors

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Abstract. Compressive sensing (CS) has triggered enormous research activity since its first appearance. CS exploits the signal's sparseness or compressibility in a particular domain and integrates data compression and acquisition, thus allowing exact reconstruction through relatively few non-adaptive linear measurements. While conventional CS theory relies on data representation in the form of vectors, many data types in various applications such as color imaging, video sequences, and multi-sensor networks, are intrinsically represented by higher-order tensors. Application of CS to higher-order data representation is typically performed by conversion of the data to very long vectors that must be measured using very large sampling matrices, thus imposing a huge computational and memory burden. In this talk we introduce Tensor Compressive Sensing (TCS)–a unified framework for compressive sensing of higher-order sparse tensors. TCS offers an efficient means for representation of multidimensional data by providing simultaneous acquisition and compression from all tensor modes. In addition, we propound two reconstruction procedures, a serial method (TCS-S) and a parallelizable method (TCS-P). We then compare the performance of the proposed method with Kronecker compressive sensing (KCS) and multi-way compressive sensing (MWCS). We demonstrate experimentally that TCS outperforms KCS and MWCS in terms of both accuracy and speed. **The talk is based on a joint paper with Qun Li and Dan Schonfeld.**
http://arxiv.org/abs/1305.5777/

Hankel-based Signal Separation of Exponential Polynomials

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Abstract. Stochastic methods such as Independent Component Analysis (ICA) are established techniques for solving the Blind Source Separation (BSS) problem. However, also deterministic methods obtain a large amount of interest in which one models the data explicitly. We present a Hankel-based method for the blind separation of exponential polynomials, i.e. sum/product of exponentials, sinusoids and polynomials (1). Related work on exponential fitting can be found in (2). The possibility of modelling/fitting the source signals deterministically can be an advantage in many applications.

We show how the observed data can be tensorized with a Hankel structure, and how a decomposition of the tensor into rank-$(L_r, L_r, 1)$ terms ensures the demixing. We discuss the existing uniqueness properties, and pay attention to the properties of the Hankel-matrix. Note that exponential polynomials also have a natural connection with Vandermonde-like structures.

In addition, we present memory and time-efficient variants in which the explicit generation of the higher-order tensor is not necessary. This is advantageous in the case of big data. These

efficient algorithms fit in a more general toolbox called Tensorlab, a new Matlab-toolbox for tensor generation/presentation/decompositions, and for complex optimization.

Reference

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(2) J.-M. Papy, L. De Lathauwer, and S. Van Huffel, "Exponential data fitting using multilinear algebra: the single-channel and multi-channel case," *Numerical linear algebra with applications*, vol. 12, no. 8, pp. 809-826, 2005.

A Trust Region Based Alternating Least-Squares Algorithm for Tensor Decompositions

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Abstract. Tensor decomposition (CANDECOMP/PARAFAC(CP)), which decomposes a given tensor as a sum of rank-one tensors, is often encountered in signal processing, hypergraph analysis and so on. Due to its simplicity, the alternating least squares (ALS) is a very popular method to solving tensor decompositions, while its convergence is not well studied (except the Tikhonov regularization based ALS (RALS method) in N. Li , S. Kindermann, C. Navasca, "Some convergence results on the Regularized Alternating Least-Squares method for tensor decomposition", *Linear Algebra and its Applications* 438(2) (2013) 796-812). In this paper, we propose a trust-region-based alternating least squares algorithm for CANDECOMP/PARAFAC(CP). Under mild assumptions, we prove that the limited point of the sequence generated by the algorithm is the stationary point of the problem. Using the classical results from numerical optimization, we suggest some effective methods to choose the trust region radius. We also report some numerical results and compare it with RALS. The results show that the new algorithm is more effcient than RALS.

An Improved ANLS Algorithm for Nonnegative Tensor Factorization

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Abstract. The Alternating Nonnegative Least Squares (ANLS) algorithm is a commonly used method for Nonnegative Tensor Factorization (NTF). However, the convergence of this method has not been proved. In this talk, we describe an algorithm for NTF that incorporates a proximal technique into the ANLS framework to enhance convergence. It is further combined with a periodic line search strategy to accelerate the convergence. The new algorithm is proved

to converge to a critical point of the NTF problem under mild conditions. We provide numerical results to compare the new method and the ANLS method.

The Maximum Eigenvalue of a Symmetric Tensor: a Polynomial Optimization Approach

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Abstract. Determining the maximum eigenvalue of a symmetric tensor is of great importance in applied mathematics and engineering, and is an intrinsically hard problem. This problem arises in various important engineering applications such as stability problem of nonlinear autonomous systems in automatic control, and provides a rich and fruit- ful interaction between multilinear algebra and global optimization. We establish some new theoretical results on the maximum eigenvalue function of an even order symmetric tensor via a polynomial optimization approach. In particular, for an mth-order n-dimensional symmetric tensor $\mathcal{A}$, we establish that the maximum eigenvalue function are ρth-order semismooth at $\mathcal{A}$ and provide explicit estimates (in terms of the order m and dimension n) of the exponent ρ. Moreover, we provide a tractable extension of Yuan's alternative theorem from matrix to the tensor setting. As a consequence, we show that the maximum eigenvalue of a symmetric tensor with suitable sign structure (or more explicitly, with essentially nonnegative coefficients) can be found by solving a single semi-definite programming problem.

This talk is based on joint works with J.M. Borwein, S. Hu, B.S. Mordukhovich, L.Q. Qi, Y. Song, L. Yao and G. Yu.

On Extreme Points of the Set of Multi-Stochastic Tensors

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Abstract. In this talk, we study the extreme points of the set of multi-stochastic tensors. Two necessary and sufficient conditions for a multi-stochastic tensor to be an extreme point are established. These conditions characterize the "generators" of multi-stochastic tensors. An algorithm to search the convex combination of extreme points for an arbitrary given multi-stochastic tensor is developed. Based on our obtained results, some expression properties for 3rd-order and n-dimensional multi-stochastic tensors ($n = 3$ and 4) are derived, and all the extreme points of the 3-dimensional and 4-dimensional triply-stochastic tensors can be produced in a simple way, respectively. As an application, a new approach for the partially filled square problem under the framework of multi-stochastic tensors is also given.

This is joint work with Rihuan Ke and Mingqing Xiao.

Tensors in Optimization Theory

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Abstract. We discuss how tensors may sometimes be useful in furthering our understanding of optimization theory, giving two examples from the speaker's recent work. The first example is that the notion of self-concordance in convex optimization may be viewed as a statement about two order-6 tensors defined via the second and third derivatives of the objective function, allowing us to deduce the somewhat curious fact that deciding self-concordance is an NP-hard problem. The second example is the recent discovery of the third and fourth order KKT conditions for constrained optimization as well as the fact that similar conditions of order five or higher do not in general exist (analogous but unrelated to the well-known result of Abel and Galois about non-existence of algebraic expressions for roots of polynomials of degree five or higher).

The second part of this talk is joint work with Shenglong Hu.

Nonnegative Tensors: Theory and Applications

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Abstract. In the literature, there are several useful and powerful results for nonnegative matrices. For instance, (i) a nonnegative matrix is irreducible if and only if its associated graph is strongly connected, and a nonnegative irreducible matrix is primitive if and only if its greatest common divisor of lengthes of all the cycles in the hypergraph is equal to one; (ii) the column sum and row sum bounds for the spectral radius of nonnegative matrices can be derived based on the transpose of nonnegative matrices. In this talk, we are interested in nonnegative tensors, and we would like to generalize these results to nonnegative tensors.

Quantum Entanglement and US-Eigenvalues of Symmetric Complex Tensors

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Abstract. Quantum entanglement of compound systems is a key resource in quantum information processing. In many practical applications it is of fundamental importance to know whether a state is entangled or not. This information is often not sufficient and it is also required to know how much a state is entangled. A useful tool to quantify the amount of entanglement

of a state is given by the so-called entanglement measures. A widely used entanglement measure is provided by the geometric measure of entanglement. However, the geometric measure of entanglement is nothing but the injective tensor norm itself. Motivated by the geometric measure of entanglement, we study complex tensor analysis problems. We first introduce the unitary eigenvalue (U-eigenvalue) of a complex tensor, the symmetric unitary eigenvalue (US-eigenvalue) of a symmetric complex tensor and the best complex rank-one approximation. Then, for symmetric tensors, we give an upper bound on the number of US-eigenvalues and count all US-eigenpairs. We indicate that a computing problem of the quantum entanglement can be equivalent to a solving problem of an algebraic system. A numerical example shows that the best complex rank-one approximation may be better than its best real rank-one approximation for a symmetric real tensor, which implies that the absolute-value largest Z-eigenvalue may be not the geometric measures of symmetric pure states.

Semidefinite Relaxations for Best Rank-1 Tensor Approximations

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Abstract. This paper studies the problem of finding best rank-1 approximations for both symmetric and nonsymmetric tensors. For symmetric tensors, this is equivalent to optimizing homogeneous polynomials over unit spheres; for nonsymmetric tensors, this is equivalent to optimizing multi-quadratic forms over multi-spheres. We propose semidefinite relaxations, based on sum of squares representations, to solve these polynomial optimization problems. Their properties and structures are studied. In applications, the resulting semidefinite programs are often large scale. The recent Newton-CG augmented Lagrangian method by Zhao, Sun and Toh is suitable for solving these semidefinite relaxations. Extensive numerical experiments are presented to show that this approach is practical in getting best rank-1 approximations.

This is joint work with Yalchin Efendiev, Juan Galvis.

Spectral Extremal Problems for Hypergraphs

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Abstract. For 2-graphs extremal spectral problems have been studied for long time, but until recently such results were not known for hypergraphs. This talk will introduce a new spectral approach to extremal hypergraph problems, and its relations to classical Turan problems for hypergraphs.

Best Rank One Approximations

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Abstract. We count critical points of the distance of a given tensor from the variety of rank one tensors and how they fit with critical points on the hyperdeterminant hypersurface. We compare this study with best rank one approximation for tensors and for matrices. We discuss the notion of Euclidean Distance Degree and its behaviour under duality.

This is joint work with S.Friedland and with J.Draisma, E.Horobet, B.Sturmfels, R.Thomas.

Hankel Tensors: Associated Hankel Matrices and Vandermonde Decomposition

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Abstract. Hankel tensors arise from applications such as signal processing. In this paper, we make an initial study on Hankel tensors. For each Hankel tensor, we associate it with a Hankel matrix and a higher order two-dimensional symmetric tensor, which we call the associated plane tensor. If the associated Hankel matrix is positive semi-definite, we call such a Hankel tensor a strong Hankel tensor. We show that an m order n-dimensional tensor is a Hankel tensor if and only if it has a Vandermonde decomposition. We call a Hankel tensor a complete Hankel tensor if it has a Vandermonde decomposition with positive coefficients. We prove that if a Hankel tensor is copositive or an even order Hankel tensor is positive semi-definite, then the associated plane tensor is copositive or positive semi-definite, respectively. We show that even order strong and complete Hankel tensors are positive semi-definite, the Hadamard product of two strong Hankel tensors is a strong Hankel tensor, and the Hadamard product of two complete Hankel tensors is a complete Hankel tensor. We show that all the H-eigenvalue of a complete Hankel tensors (maybe of odd order) are nonnegative. We give some upper bounds and lower bounds for the smallest and the largest Z-eigenvalues of a Hankel tensor, respectively. Further questions on Hankel tensors are raised.

Some New Trace Formulas of Tensors with Applications in Spectral Hypergraph Theory

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Abstract. We give some graph theoretical formulas for the trace $Tr_k(\mathbb{T})$ of a tensor $\mathbb{T}$ which do not involve the differential operators and auxiliary matrix. We also give some applications of these new trace formulas in the study of the spectra of uniform hypergraphs, including a characterization (in terms of the traces of the adjacency tensors) of the k-uniform hypergraphs whose spectra are k-symmetric, a common generalization of some previous results about the k-symmetry of the spectrum of a k-uniform hypergraph, and an answer to a question about the relation between the Laplacian and signless Laplacian spectra of a k-uniform hypergraph when k is odd. We also give a simplified proof of an expression for $Tr_2(\mathbb{T})$ and consider the expression for $Tr_3(\mathbb{T})$.

Spectral Properties of Positively Homogeneous Operators Induced by Higher Order Tensors

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Abstract. The Fredholm alternative type results are proved for eigenvalues (E-eigenvalues, H-eigenvalues, Z-eigenvalues) of a higher order tensor $\mathcal{A}$. For the positively homogeneous operators $F_{\mathcal{A}}$ and $T_{\mathcal{A}}$ induced by a higher order tensor $\mathcal{A}$, we show some relationship between the Gelfand formula and the spectral radius, and present the upper bound of their spectral radii. Furthermore, for a nonnegative tensor $\mathcal{A}$, we obtain the practical relevance for the spectral radius of the operators $F_{\mathcal{A}}$ and $T_{\mathcal{A}}$ as well as the operator norms of $F_{\mathcal{A}}$ and $T_{\mathcal{A}}$.

This is joint work with Professor Liqun Qi.

M-Tensors and Nonsingular M-Tensors

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Abstract. The M-matrix is an important concept in matrix theory, and has many applications. Recently, this concept has been extended to higher order tensors by L. Zhang, L. Qi and G. Zhou. In this talk, we establish some important properties of M-tensors and nonsingular M-tensors. An M-tensor is a Z-tensor. We show that a Z-tensor is a nonsingular M-tensor if and only if it is semi-positive. Thus, a nonsingular M-tensor has all positive diagonal entries;

and an M-tensor, regarding as the limitation of a series of nonsingular M-tensors, has all nonnegative diagonal entries. We introduce even-order monotone tensors and present their spectral properties. In matrix theory, a Z-matrix is a nonsingular M-matrix if and only if it is monotone. This is no longer true in the case of higher order tensors. We show that an even-order monotone Z-tensor is an even-order nonsingular M-tensor but not vice versa. An example of an even-order nontrivial monotone Z-tensor is also given.

This is joint work with Weiyang Ding and Liqun Qi.

Algebraic Connectivity of an Even Uniform Hypergraph

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Abstract. Hu and Qi defined the algebraic connectivity of an even uniform hypergraph in 2012 in the framework of spectral hypergraph theory. In this talk, I will report my joint work with Yuming Hua around this concept.

The Clique and Coclique Numbers' Bounds based on the H-Eigenvalues of Uniform Hypergraphs

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Abstract. In this talk, some inequality relations between the Laplacian/signless Laplacian H-eigenvalues and the clique/coclique numbers of uniform hypergraphs are presented. For a connected uniform hypergraph, some tight lower bounds on the largest Laplacian H^+-eigenvalue and signless Laplacian H-eigenvalue related to the clique/coclique numbers are given. And some upper and lower bounds on the clique/coclique numbers related to the largest Laplacian/signless Laplacian H-eigenvalues are obtained. Also some bounds on the sum of the largest/smallest adjacency/Laplacian/signless Laplacian H-eigenvalues of a hypergraph and its complement hypergraph are showed. All these bounds are consistent with what we have known when k is equal to 2.

The Methods for Solving the Spectral Radius of the Square Nonnegative Tensor

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Abstract. In this talk we will present two solution methods for finding the largest eigenvalue of general square nonnegative tensors. Our algorithms are given by using the inexact strategy of inner loop and can be implemented more easily. We give the convergence of the methods for the general nonnegative tensor. Under a certain assumption, the computing complexity of an algorithm is established. The numerical examples of algorithms presented are reported, which show the efficiency of our methods.

The Rank Decomposition and the Symmetric Rank Decomposition of a Symmetric Tensor

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Abstract. For a symmetric tensor, we show that its rank decomposition must be its symmetric rank decomposition when its rank is less than its order. Furthermore, for a symmetric tensor whose rank is equal to its order, we have that its symmetric rank is equal to its order. As a corollary, for a symmetric tensor, its rank is equal to its symmetric rank when its rank is not greater than its order. This partially gives a positive answer to the conjecture proposed by Comon, Golub, Lim and Murrain in 2008.

On the Largest Eigenvalue of a Symmetric Nonnegative Tensor

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Abstract. In this talk, some important spectral characterizations of symmetric nonnegative tensors will be reported. An algorithm for computing the largest eigenvalue of symmetric nonnegative tensors will also be discussed.

Nonnegative Tensor Decompositions: An Algorithmic Perspective

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Abstract. In many practical applications latent components to be analyzed are nonnegative and sparse and it is often preferable to take both these constraints into account to extract consistent and meaningful hidden components (sources) or factor matrices. In this talk we provide a brief survey of algorithmic and computational aspects of Nonnegative Matrix Factorization (NMF), Nonnegative Tensor Factorization (NTF) and more flexible and general Nonnegative Tucker Decompositions (NTD). Particular emphasis is given to recent developments which can considerably improve convergence speed and efficiency of existing (gradient based) algorithms. Some new algorithms for nonnegative tensor decompositions are also briefly introduced.

This is joint work with Prof. Andrzej Cichocki

Stream 6
Numerical Ordinary and Partial Differential Equations

Invited Talks

Steady and Quasi-Static Flow in a Deformable Poroelasticitic Medium

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Abstract. We are surrounded by poroelastic solid materials: natural (e.g., living tissue: plant or animal, rocks, soils) and manmade (e.g., cement, concrete, filters, foams, ceramics). Because of their ubiquity and unique properties poroelasticity materials are of interest to natural scientists, and engineers. Applications of poroelasticity include reservoir engineering, biomechanics and environmental engineering.

In this talk we present models for a steady and quasi-static flow in a saturated deformable porous medium. This is a coupled phenomenon distinguished by the interaction of a porous, deformable, elastic solid matrix and a saturating fluid which occupies and flows through its pores. We will present results on well-posedness, regularity and numerical solutions of the governing PDEs.

Periodic Boundary Conditions with Immersed Finite Elements for Interface Problems

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Abstract. This paper discusses a bilinear immersed finite element (IFE) space for solving periodic boundary conditions problems with discontinuous coefficients (interface problem). This algorithm removed periodical constraint conditions and only uses one cycle to calculate, which is less computational cost than other methods. Error analysis and numerical example are presented to demonstrate the optimal converge rate of the IFE method with periodical boundary based on Cartesian meshes, which are $O(h^2)$ in the L_2 norm, $O(h)$ in the H_1 norm.

Reverse Time Migration for Reconstructing Extended Obstacles in Planar Acoustic Waveguides

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Abstract. We propose a new reverse time migration method for reconstructing extended obstacles in the planar waveguide using acoustic waves at a fixed frequency. We prove the resolution of the reconstruction method in terms of the aperture and the thickness of the waveguide. The resolution analysis implies that the imaginary part of the cross-correlation imaging function is always positive and thus may have better stability properties. Numerical experiments are included to illustrate the powerful imaging quality and to confirm our resolution results.

An ADI Orthogonal Spline Collocation Method for the Two-Dimensional Fractional Diffusion-Wave Equation

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Abstract. We describe a new method for the approximate solution of the two-dimensional time-fractional diffusion-wave equation. In this method, orthogonal spline collocation is used for the spatial discretization. For the time-stepping, we present a novel alternating direction implicit (ADI) method based on the Crank-Nicolson method combined with the $L1$-approximation of the time Caputo derivative of order $\alpha \in (1, 2)$. A primary attraction of ADI–OSC methods is that they reduce a multidimensional problem to independent sets of one-dimensional problems in the coordinate directions similar to those arising in the OSC solution of two-point boundary value problems. These problems give rise to almost block diagonal linear systems, which can be solved efficiently using existing software.

The ADI-OSC scheme is shown to be stable and of optimal accuracy in various norms. Results of numerical experiments are presented which confirm the theoretical global error estimates and exhibit superconvergence.

Parallelizing the Time Direction: an Overview

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Abstract. Many problems in science and engineering are time dependent, and time stepping methods are used to obtain approximate solutions. If the problems are large scale, or solutions are needed in real time, it is necessary to use the computing power of parallel computers. The classical strategy to parallelize time integration is to parallelize the solution at each time step, and to advance sequentially from time step to time step. This approach however neglects an entire dimension, the time dimension, which could also be used for the parallelization. In contrast to the spatial dimensions, the time dimension has however a direction: the solution later in time depends only on the solution earlier in time, and not vice versa. It therefore seems difficult to do useful computations at a future time step, before the present time step results are known.

There are several algorithms which nevertheless try to do useful computations later in time, before fully accurate results at the present time step are available, and one of the more recent ones is based on multiple shooting: the parareal algorithm. This algorithm is using an approximation of the Jacobian on a coarse grid in the Newton iteration classically used for solving the shooting equations. After reviewing a compact convergence result for this algorithm, I will illustrate its numerical performance for several examples of systems of ordinary and partial differential equations. These examples reveal that while the algorithm performs well for diffusive problems, convergence is unsatisfactory for hyperbolic equations. I will then explain as possible remedies for this problem the Krylov parareal algorithm, and also a different time parallel method called ParaExp. I will finally show two further developments, a space-time algorithm based entirely on multigrid techniques, and a space-time algorithm based on space-time domain decomposition.

Mechanical Quadrature Methods and Their Extrapolations for Solving the First Kind Boundary Integral Equations of Stokes Equation

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Abstract. In this talk the mechanical quadrature methods are proposed and analyzed for solving the the first kind boundary integral equations of Stokes equation with both smooth boundary and piecewise linear boundary. The asymptotic expansions of the errors are proved for both of the two types of boundary. In order to obtain a higher accuracy, a Richardson extrapolation is constructed for the mechanical quadrature solution on the smooth boundary and a splitting extrapolation is constructed for the mechanical quadrature solution on the piecewise linear boundary. Numerical examples are provided to illustrate the features of the proposed numerical methods.

Modelling Absorption and Metabolism of Fatty Acid

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Abstract. The absorption and metabolism process of dietary triacylglycerol may have vital impact on the analysis of risk factors for coronary heart disease. Therefore understanding the process with a mathematical model would be very important in understanding the absorption and metabolism of dietary triacylglycerol which in turn affects the risk factors. Following the concept of a compartment theory this paper examines a mathematical model of fatty acids kinetics in plasma based on ordinary differential equations. The model is constructed through physiological knowledge and laboratory experimental data. Firstly a linear time-dependent compartment model for non-esterified fatty acid (NEFA) complex is built to describe the early event of an absorption condition. Secondly a non-linear compartment model is constructed for a specific kind of NEFA concentration based on experimental results taken from human intake of dietary supplement with steady state results. In order to estimate the unknown parameters in the model, methods of inverse problems are used with measurements and governing the kinetics. Different sets of experimental data were used to establish the unknown parameters in the mathematical model. This enables one to understand the absorption process of nutrients and provide a computational estimation for absorption rate. For the first task on the early absorption process of fatty acids, kinetic parameters of the absorption model were determined through conjugate gradient method using MATLAB. The computational results of fatty acids concentration, both in venous and arterial blood vessels, were compared with experimental data. For the second task, kinetics parameters of a nonlinear model were determined by means of an inverse problem method, based on quantum particle swarm optimization implemented in a FORTRAN program. Computational results obtained are closely conformed to the observation data.

Recent Progress in Mathematical Study of Cloak Models

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Abstract. In the June 23, 2006's issue of Science magazine, Pendry et al and Leonhardt independently published their works on electromagnetic cloaking. In Nov 2006's Science, Pendry et al demonstrated the first practical realization of such a cloak with the use of artificially structured metamaterials. Since then, there is a growing interest in using metamaterials to construct invisibility cloaks. In this talk, I'll focus on the mathematical study of those cloak models. Numerical simulations in both frequency domain and time domain will be presented.

The Efficient Splitting Characteristic Method for Aerosol Transport Problems in Environment

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Abstract. Global climate change and warming in atmosphere have been widely recognized. As one of most important constituents, aerosols have a direct radiative forcing by scattering and absorbing solar and infrared radiation in atmosphere, while they have an indirect radiative forcing associated with the changes in cloud properties by decreasing the precipitation efficiency of warm clouds. Numerical simulation has been playing a key role in the study of aerosol processes and aerosol concentration distributions in the atmospheric environment prediction and the air quality control. Aerosol transport model in atmosphere is a complex multi-component system that involves several physical and chemical processes, such as emission, advection, dispersion, deposition and aerosol processes including condensation/evaporation, coagulation and aerosol chemistry, and the area it studies usually covers a large region. In this study, we develop the efficient splitting characteristic method for the aerosol transports in environment. We propose the characteristic method to solve the transport process in the spatial dynamical system by combining with the splitting technique. The method can efficiently compute the prediction of multi-component aerosol transport dynamics in high-dimensional domains with a large range of aerosol concentrations and for different types of aerosols including aerosols containing sea salt component. Numerical experiments show the computational efficiency of the method comparing with other algorithms. The developed algorithm can be applied for the large scale predictions of multi-component aerosol in multi regions and levels in environment.

Optimal Control of Stochastic Flow Using Reduced Order Modeling

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Abstract. The most challenging problem for dealing with optimal control problem of stochastic flow is the formidable computational complexity. In the lecture, we will explore a low-dimensional approximation to reduce the degrees of freedoms of the control system. Several methods, including POD (proper orthogonal decomposition), CVT (centroidal Voronoi tessellation), CVOD (CVT-based POD) and PCE (polynomial chaos expansion), are considered and compared to form our reduced-order modeling (ROM). Numerical tests of various situations are performed to validate our conclusion.

Conforming and Divergence-Free Stokes Finite Elements

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Abstract. In this talk, we discuss three families of conforming finite elements for the two dimensional Stokes problem that produce exactly divergence-free approximations on very general triangulations. The construction of these elements is guided by two discrete smooth de Rham complexes ("Stokes complexes"). Extensions to the three dimensional setting will also be discussed.

Gradient Based Dimension Reduction Approach for Stochastic Partial Differential Equations

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Abstract. Dimension reduction approach is considered for uncertainty quantification, where we use gradient information to partition the uncertainty domain into "active" and "passive" subspaces, where the "passive" subspace is characterized by near zero variance of the quantity of interest. We present a way to project the model onto the low dimensional "active" subspace and solve the resulting problem using conventional techniques. We derive rigorous error bounds for the projection algorithm and show convergence in L^1 norm.

Multigrid Methods for Saddle Point Problems

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Abstract. We will present multigrid methods for saddle point problems that are uniformly convergent in the energy norm. Examples include saddle point problems arising from mixed finite element discretizations of Stokes, Lamé and Darcy systems.

This is joint work with Susanne Brenner, Hengguang Li and Duk-Soon Oh.

Improving Time-Stepping Numerics for Weakly Dissipative Systems

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Abstract. In this talk I will address the stability & accuracy of CNLF time-stepping scheme and a modification of Robert-Asselin time-filters for numerical models of weakly diffusive evolution systems. This is motivated by the vast number of applications, e.g., the meteorological equations, and coupled systems with dominating skew symmetric coupling (ground-water surface-water).

Variable-Coefficient Space-Fractional Diffusion Equations: Mathematical Analysis and Fast Numerical Solution

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Abstract. Fractional differential equations, which describe phenomena exhibiting anomalous diffusion that cannot be modeled accurately by second-order diffusion equations, raise mathematical and numerical difficulties that have not been encountered in the analysis and numerical simulation of second-order differential equations. The wellposedness of a Galerkin weak formulation to space-fractional diffusion equations with a constant diffusivity coefficient has been proved. Subsequently, error analysis for corresponding finite difference methods, finite element methods, discontinuous Galerkin methods, and spectral methods was derived, under the same assumption of a constant diffusivity coefficient.

In this talk we present a counterexample which shows that the Galerkin formulation loses coercivity in the context of variable-coefficient fractional differential equations. Hence, the previous results cannot be extended to variable-coefficient problems. We outline an alternative approach to prove the existence and uniqueness of the classical solution to a class of variable-coefficient conservative fractional differential equation and characterize the solution in terms of the classical solutions to second-order differential equations. We present a Petrov-Galerkin formulation to the problem and show that the formulation is weakly coercive and well posed.

In this talk we also address the issues on the development of faithful and efficient numerical methods for space-fractional partial differential equations. Because of the nonlocal property of fractional differential operators, the numerical methods for fractional diffusion equations often generate dense or even full coefficient matrices. Consequently, the numerical solution of these methods often require computational work of $O(N^3)$ per time step and memory of $O(N^2)$ for where N is the number of grid points. We present fast numerical methods that have computational cost of $O(Nlog^2N)$ per time step and memory of $O(N)$, while retaining the same accuracy and approximation property as the regular finite difference method with Gaussian elimination. Numerical experiments show that to achieve the same accuracy, the new method has a significant

reduction of the CPU time from more than 2 months consumed by a traditional finite difference method to 5.74 seconds for a problem with 36,000 grid points on a work station with 128GB memory. This demonstrates the utility of the method.

Weak Galerkin Finite Element Methods

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Abstract. In this talk, the speaker will introduce the basic principle of weak Galerkin finite element methods for partial differential equations. The second order elliptic equations shall be used as a model problem for presenting the basic concept of weak Galerkin. In particular, a comparison with existing finite element methods will be made. The speaker will then demonstrate how weak Galerkin can be applied to other PDEs, such as the Stokes equations, the biharmonic and Maxwells equations. This talk should be accessible to all audience with graduate level training in computational mathematics.

A Hyper-Spherical Sparse Grid Approach for High-Dimensional Discontinuity Detection

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Abstract. High-dimensional discontinuity detection is significantly important to several areas of science and engineering. For example, in uncertainty quantification (UQ), it is directly related to risk assessment and predicting rare events. More generally, in an N-dimensional Euclidean space, the location of the discontinuity is generally an N-1-dimensional manifold, and therefore, the most difficult challenge is to accurately and efficiently represent such manifold. Conventional adaptive sparse-grid hierarchical interpolation has been employed to characterize such manifolds, however, the mesh refinement densely places grid points around the discontinuity, and fails to "sparsely" represent the N-1 dimensional manifold.We propose a novel method for identifying jump discontinuities in high dimensional spaces by incorporating a hyper-spherical coordinate system (HSCS) into the sparse-grid approximation framework. The basic idea is to transform the Cartesian coordinate system to an N-dimensional HSCS and treat the manifold as the N-1 dimensional function in the subspace constituted by the N-1 angle coordinates. Then a sparse-grid approximation can be constructed in the subspace where the function value at each grid point is estimated by solving a nonlinear equation with use of the bisection or Newton method. This novel technique identifies the discontinuity with a reduced number of sparse grid points compared to existing methods. Rigorous analysis of the computational complexity of our approach will be presented and several numerical examples will be used to show the increased efficiency and accuracy of our approach for detecting the discontinuities.

Hybrid Stress Finite Element Analysis: Theory and Applications

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Abstract. Hybrid stress finite element method (HSFEM), pioneered by T.H.H. Pian (1964), is known to be an efficient approach in the elasticity analysis to improve the performance of the standard 4-node quadrilateral displacement scheme while preserving the privileges of the latter one. This talk presents an overview of the method. The contents include: uniform stability and convergence of HSFEM; 3D extension; and some applications to elastodynamics, stochastic elasticity, and multiscale elasticity.

On a Robin-type Nonoverlapping Domain Decomposition Preconditioner

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Abstract. In this talk, we shall present a new Robin-type nonoverlapping domain decomposition preconditioner. The unknown variables to be solved in this preconditioned algebraic system are the Robin transmission condition on the interface, which are different from the well-known DD methods like substructuring nonoverlapping DD method and FETI method. By choosing suitable parameter on each subdomain boundary and using the tool of energy estimate, for the second-order elliptic problem, we prove that the condition number of the preconditioned system is $C(1 + log(H/h))^2$, where H is the coarse mesh size and h is the fine mesh size. Numerical results shall be given to illustrate the efficiency of our DD preconditioner.

This talk is based on a joint work with Yongxiang Liu.

A New Class of Finite Element Methods: Weak Galerkin Methods

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Abstract. When the classic continuous finite element methods cannot meet the needs of modern computational techniques such as hp adaptive and hybrid meshes, discontinuous piecewise polynomials are used in the finite element procedures.

This presentation will study the finite element methods that use totally discontinuous approximation functions. Discontinuous Galerkin (DG) methods are such kind methods including

IPDG methods, LDG methods and HDG methods. DG methods enforce the continuity of the approximation solutions cross elements by tuning penalty parameters or introducing additional equations. The weak Galerkin (WG) finite element method provides a framework for handling discontinuous functions. This general framework will provide a platform for the imagination of deriving new methods. A successful example will be discussed in the presentation.

A Hybrid Adaptive Sparse-Grid Method for High-Dimensional Zakai Equation

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Abstract. We propose a hybrid approach for high-dimensional Zakai equations in order to overcome the instability issue of extended Kalman filter and particle filter in estimating the density function of the state of the dynamic system of interest. The Zakai equation is discretized using a splitting-up approximation in the temporal domain. In the potentially high-dimensional spacial domain, an adaptive sparse-grid (ASG) method is used to approximate the desired density function such that the so-called "curse of dimensionality" can be alleviated to some extent. In addition, an adaptive high-probabilit domain detection approach is proposed based on particle filter technique in order to reduce the volume of the domain in which the ASG approximation is constructed. Several numerical examples shows that our method is more stable and efficient than particle filter and conventional grid-based method for Zakai equations.

Polynomial Preserving Recovery for Gradient and Hessian including boundary

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Abstract. As an alternative to Superconvergent patch recovery (SPR, due to Zienkiewicz-Zhu), Polynomial preserving recovery (PPR, due to Zhang-Naga) has been widely accepted by the scientific community, which is evidenced by its implementation into COMSOL Multiphysics, a fast developing commercial software. In this talk, some recent development of polynomial preserving recovery (PPR) will be discussed with particular interests on the boundary strategy and Hessian recovery.

A Mixed Hybrid Discontinuous Galerkin Method for Convection-Diffusion Interface Problem

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Abstract. Interface problems arise from multi-materials (solid, liquid and gas), multi-physics, and many advanced technologies and engineering applications. These problems can be modeled generally by partial differential equations with discontinuities and singularities in the coefficients and the solutions. The standard numerical methods designed for smooth solutions usually perform poorly for these problems. To overcome this difficulty, the immersed boundary method (IBM) was proposed by Peskin in 1977 to model blood flow in the heart . Since then, many other numerical methods, such as the immersed interface method (IIM), the decomposed immersed interface method (DIIM), the level set method, the ghost fluid method, and the matched interface and boundary (MIB) method, have been developed. There are two classes of finite element methods for interface problems: *fitted interface*and *unfitted interface* methods. In fitted interface methods, the finite element mesh is designed to align with the interface. And in unfitted interface methods, the finite element mesh is independent on the interface geometry and the interface usually cuts through elements, then the unstructured meshes can be applied.

The discontinuous Galerkin (DG) method has a great advantage for solving the interface problems. In this work, we propose a mixed hybrid discontinuous Galerkin (MHDG) finite element method for the convection-diffusion interface problem with non-homogeneous jump conditions. By introducing the Lagrange multipliers to approximate the traces of the solution on element boundaries, the MHDG method can reduce significantly the global degrees of freedom in comparing with the DG method. After the approximated traces are computed, the problem can be solved locally in element level. The consistence, conservation, existence and uniqueness of the MHDG scheme are proved. Numerical examples are presented to show the performance of the proposed method.

Contributed Talks

A Two-Grid Finite Volume Element Method for a Nonlinear Parabolic Problem

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Abstract. A two-grid algorithm is presented and discussed for a finite volume element method to a nonlinear parabolic equation in a convex polygonal domain. The two-grid algorithm consists of solving a small nonlinear system on a coarse-grid space with grid size H and then solving a resulting linear system on a fine-grid space with grid size h. Error estimates are derived with the H^1-norm $O(h + H^2)$ which shows that the two-grid algorithm achieves asymptotically optimal approximation as long as the mesh sizes satisfy $h = O(H^2)$. Numerical example is presented to validate the usefulness and efficiency of the method.

Efficient Solvers of Discontinuous Galerkin Discretization for the Cahn-Hilliard Equations

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Abstract. In this paper, we develop and analyze a fast solver for the system of algebraic equations arising from the local discontinuous Galerkin (LDG) discretization and implicit time marching methods to the Cahn-Hilliard (CH) equations with constant and degenerate mobility. Explicit time marching methods for the CH equation will require severe time step restriction ($\Delta t \sim O(\Delta x^4)$), so implicit methods are used to remove time step restriction. Implicit methods will result in large system of algebraic equations and a fast solver is essential. The multigrid (MG) method is used to solve the algebraic equations efficiently. The Local Mode Analysis method is used to analyze the convergence behavior of the linear MG method. The discrete energy stability for the CH equations with a special homogeneous free energy density $\Psi(u) = \frac{1}{4}(1-u^2)^2$ is proved based on the convex splitting method. We show that the number of iterations is independent of the problem size. Numerical results for one-dimensional, two-dimensional and three-dimensional cases are given to illustrate the efficiency of the methods. We numerically show the optimal complexity of the MG solver for $\mathcal{P}^1$ element. For $\mathcal{P}^2$ approximation, the optimal or sub-optimal complexity of the MG solver are numerically shown.

Numerical Approximation of Second Order Wave Equations by Newmark Scheme

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Abstract. We review and compare widely used time-stepping methods for solving the second order wave equation. We identify their main properties and investigate their relationship. The emphasis is on the Newmark scheme which has been used extensively in applications. We present a rigorous stability analysis for the scheme and derive sharp stability results. A convergence analysis is carried out where a discontinuous Galerkin discretization in space is used. Optimal a priori error estimates are obtained. For sufficiently smooth solutions, we demonstrate that the maximal error in the L^2-norm error over a finite time interval converges optimally as $O(h^{p+1}+k^s)$, where p denotes the polynomial degree, $s = 1$ or 2, h the mesh size, and k the time step.

Optimized Schwarz methods with unsymmetric domain decomposition

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Abstract. Among the many domain decomposition methods, optimized Schwarz methods (OSM) can enhance the convergence of subdomain iterations remarkably. The influence of the domain decomposition geometry on the convergence and the optimized parameters is however not yet fully studied; for first steps, see [Gander and Xu, Optimized Schwarz algorithm with two-sided transmission conditions in an unsymmetric domain decomposition, talk on DD22, Lugano, 2013] for two-sided transmission conditions. In this talk, we continue our research on OSM for unsymmetric domain decompositions. We derive optimized Robin and optimized 2nd order transmission conditions. Our theoretical analysis on the asymptotic performance of the OSMs with the new transmission conditions shows that they perform better than the ones obtained from the infinite domain decomposition analysis in [M. Gander, Optimized Schwarz Methods, SIAM J. Numer. Anal.,22(2) 2006: 699-731]. We illustrate our theoretical results with numerical experiments.

An Efficient Numerical Method for the Biharmonic Equation by Weak Galerkin Finite Element Methods on Generic Polygonal or Polyhedral Meshes

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Abstract. This talk will present a new and efficient numerical method for the biharmonic equation by using weak Galerkin (WG) finite element methods. This WG finite element scheme is based on a variational form of the biharmonic equation that is equivalent to the usual semi H^2 norm. The speaker shall introduce second order weak partial derivatives and their discrete analogues in a carefully constructed finite element space consisting of discontinuous functions defined on polygonal or polyhedral elements and their boundaries. These discrete second order weak partial derivatives shall be used to construct a WG finite element scheme for the biharmonic equation. The resulting WG finite element scheme is symmetric, positive definite, and parameter-free. An optimal order error estimate in a discrete H^2 norm is established for the corresponding WG finite element solutions. The speaker will also discuss some error estimates in the usual L^2 norm. Numerical results are to be presented to confirm the mathematical convergence theory. The convergence theory is based on some technical estimates for functions in the weak finite element space, including Poincare-type inequalities and certain norm equivalence.

Maximum Principles for $P1$-Conforming Finite Element Approximations of Quasi-Linear Second Order Elliptic Equations

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Abstract. This paper derives some discrete maximum principles for $P1$-conforming finite element approximations for quasi-linear second order elliptic equations. The results are extensions of the classical maximum principles in the theory of partial differential equations to finite element methods. The mathematical tools are based on the variational approach that was commonly used in the classical PDE theory. The discrete maximum principles are established by assuming a property on the discrete variational form that is of global nature. In particular, the assumption on the variational form is verified when the finite element partition satisfies some angle conditions. For the general quasi-linear elliptic equation, these angle conditions indicate that each triangle or tetrahedron needs to be $\mathcal{O}(h^\alpha)$-acute in the sense that each angle α_{ij} (for triangle) or interior dihedral angle α_{ij} (for tetrahedron) must satisfy $\alpha_{ij} \leq \pi/2 - \gamma h^\alpha$ for some $\alpha \geq 0$ and $\gamma > 0$. For the Poisson problem where the differential operator is given by Laplacian, the angle requirement is the same as the existing ones: either all the triangles are non-obtuse or each interior edge is non-negative. It should be pointed out that the analytical tools used in this paper are based on the powerful De Giorgi's iterative method that has played important roles in the theory of partial differential equations. The mathematical analysis itself is of independent interest in the finite element analysis.

Workshop 1
Computational and Mathematical Finance

Invited Talks

Mean Field Games and Mean Field Type Control

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Abstract. Mean field theory has raised a lot of interest in the recent years, since their independent introduction by Lasry-Lions and Huang-Caines-Malham. The applications concern approximating an infinite number of players with common behavior by a representative agent. This agent has to solve a control problem perturbed by a field equation, representing in some way the behavior of the average infinite number of agents. The mean-field term can influence the dynamics of the state equation of the agent as well as his objective functional. In the mean field game, the agent cannot influence the mean field term, considered as external. Therefore, he solves a standard control problem, in which the mean field term acts as a parameter. In this context one looks for an equilibrium, which means that the mean field term is the expected value of the state behavior of the individual agent. The equilibrium is the core of the mathematical difficulty. In the mean-field type control problem, the agent can influence the mean field term. The problem is purely a control problem, however more elaborate than the standard control theory problem. Indeed the state equation, contains also the probability distribution of the state and thus is of Mc Kean-Vlasov type. The objective of this talk is to describe the major approaches of the two types of problems and more advanced questions for future research.

Local Properties of Behavioral Analysis in Finance

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Abstract. In finance, it has been long realized that the expected utility theory cannot explain many "irrational behavior," which is nonlinear in nature. Theories and methodologies have been developed for characterizing such non-linear behavior and dealing with portfolio optimization problem with the non-linear criteria. Among them are Yaari's axiomatic approach, Quiggin's rank-dependent expected utility, Machina's smoothness analysis, and Zhou's quantile approach to portfolio selection. We take a different perspective; the nonlinear nature makes sensitivity analysis, in particular, perturbation analysis, a suitable tool in exploring the nature of the problem. Our recent research explores the local properties in non-linear behavior analysis and their relations to the global ones.

One important property we discovered is the so called mono-linearity, which says that Yaari's representation in fact maintains some local linearity. With the mono-linearity, we proceed in three directions. 1. Just like in perturbation analysis, the mono-linearity allows use sample path based derivatives as the unbiased estimate of the performance gradient; therefore, we develop algorithms for performance optimization in portfolio management and develop theory for it. The results are consistent with those with Zhou's; and the method can also be applied to new problems. 2. The mono-linearity explains, in one angle, why Yaari's theory cannot explain some paradoxes, and we developed new axioms to extend Yaari's axiomatic approach; in particular, we proved that the famous independent axiom can be replaced by a local linear axiom, and thus simplified the theory. 3. bvWe study other non-liner behavior when the mono-linearity does not hold; e.g., the theory with disappointment and more.

Interconnected Balance Sheets, Market Liquidity, and the Amplification Effects in a Financial System

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Abstract. This paper investigates the amplification effects of a financial system to develop individual defaults to a systemic catastrophe. In our model, the financial institutions interconnect via two mutually stimulating channels: their balance sheets are linked directly by holding debt claims against each other; they share the market liquidity to liquidate assets to meet debt liabilities when they face distress. Formulating the problem as an optimization with equilibrium constraints characterizes how the topological structures of the system and asset liquidation interact with each other to amplify the systemic risk. Two multipliers, network multiplier and liquidity multiplier, are identified to capture the above amplification effects. The model has a significant computational advantage and can be solved efficiently through the linear-complementarity-technique based fixedpoint algorithm. This research also builds up a close connection between the study of financial systemic risk and the literature of stochastic network. Furthermore, we examine some policy implications yielded from the numerical experiments on the data of European Banking Authority 2013 stress tests.

This is a joint work with David D. Yao (Columbia) and Xin Liu (CUHK).

A New Kind of Low-Risk Option

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Abstract. In this paper, it is assumed that there exists a complete and continuous financial market. In this market, the pricing of a new option with payoff $(\sqrt{KS_T} - K)^+$ is explored. This kind of option has a lower payment than the standard one, thus it can meet the requirements of risk-averse investors. Especially during the financial crisis, options with lower risk will become more and more popular. By means of Martingale method as well as the Girsanov theorem, this paper gives a succinct pricing formula for this kind of European exotic call option.

On Modeling Economic Default Time: A Reduced-Form Model Approach

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Abstract. In the aftermath of the global financial crisis, much attention has been paid to investigating the appropriateness of the current practice of default risk modeling in banking, finance and insurance industries. A recent empirical study by Guo et al. (2008) shows that the time difference between the economic and recorded default dates has a significant impact on recovery rate estimates. Guo et al. (2011) developed a theoretical structural firm asset value model for a firm default process that embeds the distinction of these two default times. In this paper, we assume the market participants cannot observe the firm asset value directly and we developed reduced-form models for characterizing the economic and recorded default times. We derive the probability distributions of these two default times. Numerical experiments with empirical data are given to demonstrate the proposed models.

Investment Decision without Time Consistency

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Abstract. An investment problem in a dynamic financial market can be formulated as a control problem. When the objective of the investment problem is good enough, the optimal trading strategy for the investment problem starting from time 0 is still optimal for the same investment problem starting from any future time (i.e., the optimality is time consistent), hence we can use dynamic programming to find the optimal trading strategy. In this talk, I will show some examples where the "optimal" trading strategy determined at time 0 is not optimal for the problem in the future. I will then re-define the solution for this type of control problem, and apply the result to the mean-variance investment problem in a continuous time financial market.

Numerical Algorithms for R&D Stochastic Control Models

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Abstract. We consider the optimal strategy of R&D expenditure adopted by a firm that engages in R&D to develop an innovative product to be launched in the market. The firm faces with technological uncertainty associated with the success of the R&D effort and market uncertainty of the stochastic revenue flow generated by the new product. Our model departs from most R&D models by assuming that the firm's knowledge accumulation has impact on the R&D progress, so the hazard rate of arrival of R&D success is no longer memoryless. Also, we assume a finite life span of the technologies that the product resides on. In this paper, we propose efficient finite difference schemes that solve the Hamilton-Jacobi-Bellman formulation of the resulting finite time R&D stochastic control models with an optimal control on R&D expenditure and an optimal stopping rule on the abandonment of R&D effort. The optimal strategies of R&D expenditure with varying sets of model parameters are analyzed. In particular, we observe that R&D expenditure decreases with firm's knowledge stock and may even drop to zero when the accumulation level is sufficiently high.

This is joint work with Prof. Yue Kuen Kwok.

H-J-B Equations of Optimal Consumption-Investment and Verification Theorems

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Abstract. We consider a consumption-investment problem on infinite time horizon maximizing (discounted) expected HARA utility for a general incomplete market model. Based on dynamic programming approach, we derive the relevant H-J-B equation and show the existence and uniqueness of the smooth solution to the equation. By using the solution we construct the optimal consumption rate and portfolio strategy and then prove the verification theorems under certain general settings.

"True Identification Properties" of Change-point Estimators

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Abstract. In this presentation, a penalized likelihood approach for the change point problem is discussed. A new penalty function called modified unbounded penalty is introduced to pursue consistent estimation in the number of change points and their locations and sizes. The asymptotic properties of the estimation from the modified unbounded penalty are compared with commonly used penalties, including Lasso, Scad, and Bridge. New results of the asymptotic theory for the set of local solutions are presented. Evidence from simulation results is also presented.

Indefinite Mean-Field Stochastic Linear-Quadratic Optimal Control with Application to Dynamic Mean-Variance Portfolio Selection

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Abstract. This paper is concerned with the discrete-time indefinite mean-field linear-quadratic (MF-LQ) optimal control problem. The cost functional consists of not only quadratic but also linear terms of system states and control inputs, which is quite general and includes the dynamic multi-period mean-variance portfolio selection problem as a special case. Due to the nonseparability of the problem, the often used dynamic-programming-based method fails to work. By a method of completing the square and a modified backward recursive technique, we find that both the well-posedness and the solvability of the MF-LQ problem are equivalent to the solvability of two coupled constrained generalized difference Riccati equations and a constrained linear recursive equation. Different from the definite one, the indefinite optimal control has five degrees of freedom. We characterize the optimal control set completely, and obtain a set of necessary and sufficient conditions on conventional dynamic multi-period mean-variance portfolio selection. It is found that though the optimal portfolio selection strategy is not unique, the optimal expected wealth and efficient frontier can be uniquely determined. Similar results are obtained for dynamic multi-period mean-variance portfolio selection with intertemporal restrictions; and when the return rates of the risky securities are nondegenerate, the results of this paper reduce to those in existing literature.

Weak Convergence Methods for Approximation of Path-Dependent Functional

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Abstract. This paper develops approximation methods for path-dependent functionals, which have been used in many applications involving path-dependent objective functions. By a first glance, the problem may appear as a standard approximation of a stopping time problem using traditional techniques. Nevertheless, a closer scrutiny would reveal that the problem under consideration is far more challenging and difficult. The difficulty is mainly because the traditional dynamic programming approach falls apart, not to mention any hope for a closed-form solution or any viable numerical PDE methods. This paper focuses on approximation methods in Monte Carlo simulations. To the best of our knowledge, convergence analysis is

available only in few special cases due to the complexity of the nature of path dependence. In contrast to the traditional approach, this work provides a non-traditional convergence method in Monte Carlo analysis, and establishes a general framework for the convergence analysis using the Markov chain approximations. In particular, the approach is based on actual computations under the Skorohod topology. Some examples such as the approximation of discretely monitoring barrier option are considered.

Numerical Solution of Fractional Black-Scholes Equations and Inequalities Arising in Pricing European and American Options under a Levy Process

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Abstract. In this talk I will present some of our recent results on solving a fractional-order differential linear complementarity problem (LCP) or variational inequality governing American option valuation when an underlying stock price follows a geometric Levy process. (European option pricing is a special case.) We will first propose a penalty method for the LCP, yielding a nonlinear fractional-order Black-Scholes equation (FBSE) approximating the LCP. We show that the solution to the nonlinear FBSE converges exponentially to that of the LCP, depending on the parameters used in the penalty method. We will then construct a 2nd-order finite difference scheme for the FBSE and prove that the finite difference method is stable and convergent. Extensions of these methods to 2-dimensional problem, i.e., problems of pricing options with 2 underlying assets, will be discussed as well. Numerical examples will be presented to demonstrate the rates of convergence of both the penalty method and the finite difference scheme. Numerical results will also show the usefulness of the methods for pricing European and American options of this type.

Calibration of Financial Models

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Abstract. Many financial models involve parameters which are chosen to help the model match market data. Issues that frequently arise include the choice of parameters, building problem characteristics into the choice of parameters, the stability of the parametrisation as the data changes, sparseness of the available data depending on the market and tractability so the model can rapidly respond to changes. An example is using semidefinite programming to parametrise covariance/correlation sensitive products, such as swaptions.

Myth and Insights on Funding Valuation Adjustment

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Abstract. Funding valuation adjustment (FVA) is about the valuation adjustment for funding costs and funding risks in securities pricing, and the issue has been under heated debates for years. In this talk, we will present our view on whether and how to make funding valuation adjustment.

Forward and Future Implied Volatility

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Abstract. We address the problem of defining and calculating forward volatility implied by option prices when the underlying asset is driven by a stochastic volatility process. We examine alternative notions of forward implied volatility and the information required to extract these measures from the prices of European options at fixed maturities. We then specialize to the SABR model and show how the asymptotic expansion of the bivariate transition density in Wu 2012 allows calibration of the SABR model with piecewise constant parameters and calculation of forward volatility. We then investigate empirically whether current option prices at multiple maturities contain useful information in predicting future option prices on the EUR/USD,GBP/USD, and USD/JPY exchange rates. We find that model-based forward volatility extracts this predictive value. Moreover, we find that model-based forward volatility extracts this predictive information better than a standard "model-free" measure of forward volatility and better than spot implied volatility. The enhancement to out-of-sample forecasting accuracy gained from model-based forward volatility is greatest at longer forecasting horizons.

Stochastic Filtering and Optimal Control

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Abstract. In this talk, we first introduce a few examples which calls for the combined study of stochastic filtering and optimal control. Then, we will present some results on stochastic maximum principle under partial information. After that, we will introduce the filtering models including the one based on the analysis of financial ultra-high frequency data. Finally, for the solution to these filtering problems, we will introduce their numerical approximations based on branching interacting particle systems.

Valuing Contingent Options

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Abstract. Motivated by the valuation problem of Guaranteed Minimum Death Benefits in various equity-linked products, we consider valuing contingent options. At the time of death, a benefit payment is due. It may depend not only on the price of a stock or stock fund at that time, but also on prior prices. The problem is to calculate the expected discounted value of the benefit payment. Because the distribution of the time of death can be approximated by a combination of exponential distributions, it suffices to solve the problem for an exponentially distributed time of death. The stock price process is assumed to be the exponential of a Brownian motion or a Brownian motion plus an independent compound Poisson process whose upward and downward jumps are modeled by an exponential distributions. In this talk, results for various contingent options will be presented.

This talk is based on a joint paper with Hans U. Gerber and Elias S. W. Shiu.

Some Recent Results on Time-Inconsistent Optimal Control Problems

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Abstract. Time-inconsistency appears in various optimal control problems, mainly due to people's time-preferences and risk-preferences. Mathematically, to describe people's time-preferences, one can adopt general discounting in the cost/payoff functional; to describe people's risk-preferences, one can include conditional expectation in some nonlinear way in the cost/payoff functional. In this talk, we present some recent works for time-inconsistent optimal control problems. The major goal is to fine time-consistent equilibrium controls/strategies

Numerical Solutions of BSDEs, a Finite Transposition Method

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Abstract. In this work, we present a new numerical method for solving BSDEs. Our method can be viewed as an analogue of the classical finite element method solving deterministic PDEs.

This is joint work with Dr. Penghui Wang.

Contributed Talks

Modified Neumann Series for Some Classes of Integral Equations

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Abstract. One can prove that boundary value problems lead to Fredholm-type integral equations and there is also a strong connection between ordinary differential equations and the Volterra-type integral equations. In turn, integral equations are normally easier to solve. Nonlinear Fredholm integral equation of the second kind are usually classified as:

$$x(t) = g(t) + \lambda \int_a^b K(t,s,x(s))ds, \quad t \in [a,b], g \in C[a,b] \text{ and } K \in C\big([a,b]^2 \times \mathbb{R}\big). \tag{1}$$

Similarly the nonlinear Abel-Volterra integral operators of the second kind are represented by:

$$x(t) = g(t) + \int_0^t \frac{K(t,s,x(s))}{(t-s)^\alpha} ds, \quad 0 \leqslant \alpha < 1, \quad t \in [0,b]. \tag{2}$$

Equations (1, 2) can be regarded as operator equations $A : C[I] \longmapsto C[I], I \subseteq \mathbb{R}$, where $x - Ax = g$, which possess a unique continuous solution provided that A is a contraction that is; $\|A\| < 1$. At least from a theoretical point of view the Neumann series obtained from Picard's iteration defined by $x_{n+1} := Ax_n + g$, converges to x as $n \to \infty$. For some equations though, the evaluations of Picard's iterations is overwhelming. It has been shown, for example, that one of the famous equations of Lighthill can be converted to:

$$h(t) = 1 - \frac{\sqrt{3}}{\pi} \int_0^t \frac{s^{\frac{1}{3}} h^4(s)}{(t-s)^{\frac{2}{3}}} ds. \tag{3}$$

Substituting $h_0(t)$ by 1 and employing Picard's iterations one obtains the n^{th} partial sums of the Neumann series for equation (3) as:

$$h_n(t) = \sum_{i=0}^{\mathbb{N}_n} a_i t^{i(1-\alpha)}, \quad \alpha = \frac{2}{3}, \tag{4}$$

for some positive integer N_n whose value can significantly be larger than n. For example $N_2 = 5, N_3 = 21, \ldots N_9 = 87381, \ldots$. As an alternative we define our modified Neumann series by:

$$S_n(t) = \sum_{m=0}^{n} a_m t^{m(1-\alpha)}, \tag{5}$$

using only the first n terms of the partial sums. One can easily find several hundreds of coefficients a_ms in equation (5) using a simple Mathematica or Maple program. We note that $S_n(t)$ is a subsequence of the convergent Neumann sequence and coverages to x on some interval $[0, r_0]$, $r_0 \leq b$, b given by equation (1) or (2). The small interval of convergence $[0, r_0]$ can be extended quite significantly, in most practical cases, using nonlinear accelerators. Modified Picard iteration can be used as an alternative to quadrature methods that have some practical limitations. After analyzing some theoretical aspect of the method, some examples in different categories of practical importance will be solved to demonstrate the practically of the method.

Predictor-Corrector Approach for Pricing American Options under the Finite Moment Log-Stable Model

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Abstract. This paper investigates the pricing of American options under the FMLS (finite moment log-stable) model. Under the FMLS model, the price of American-style options is governed by a highly nonlinear FPDE (fractional partial differential equation) system, which is much more complicated to solve than the corresponding B-S (Black-Scholes) system, with difficulties arising from the semi-globalness of the fractional operator, in conjunction with the nonlinearity associated with the early exercise nature of American-style options. Albeit difficult, in this paper, we propose a new predictor-corrector scheme based on the spectral-collocation method to solve for the prices of American options under the FMLS model. In the current approach, the non-linearity of the pricing system is successfully dealt with using the predictor-corrector framework, whereas the non-localness of the fractional operator is elegantly handled. Various numerical experiments suggest that the current method is fast and efficient, and can be easily extended to price American-style options under other fractional diffusion models. Based on the numerical results, we have also examined quantitatively the influence of the tail index on American put options.

On Reduced Form Intensity-based Model with Trigger Events

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Abstract. Corporate defaults may be triggered by some major market news or events such as financial crises or collapses of major banks or financial institutions. With a view to develop a more realistic model for credit risk analysis, we introduce a new type of reduced-form intensity-based model that can incorporate the impacts of both observable trigger events and economic environment on corporate defaults. The key idea of the model is to augment a Cox process with trigger events. Both single-default and multiple-default cases are considered in this paper. In the former case, a simple expression for the distribution of the default time is obtained. Applications of the proposed model to price defaultable bonds and multi-name Credit Default Swaps (CDSs) are provided.

This is joint work with W.K.Ching (HKU), T.K.Siu (City Univ. London), Harry Zheng (Imperial College).

Fractal Dimensional Analysis of Financial Time Series

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Abstract. Fractal dimension analysis has been introduced into financial time series by Mandelbrot and Peters. To distinguish between the randomness and determinism of the financial information a predictability index for various Indices in a financial market is proposed. Regarding the stochastic market dynamics following fractional Brownian motion, the predictability is quantified using fractal dimension analysis of the time series for each of the considered indices. These days we witness unprecedented volatility in the exchange rate. We test for fractional dynamic behavior in a 1-month forward exchange rate of USD against other Asian countries and intra-Asian countries too. We may also consider Gold Price against USD. The fractal dimension is calculated from Hurst exponent H using the relation: $D = 2 - H$ where H is a Hurst exponent.

Projected Triangular Decomposition Methods for Pricing American Options

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Abstract. Numerical pricing of American options with Heston stochastic volatility model is considered. The complementarity problem with a two-dimensional parabolic partial differential operator is discretized by the Craig-Sneyd alternative direction implicit scheme, and the resulted linear complementarity problems at each time step are solved by the projected triangular decomposition methods, which are constructed as an extension of the classical Brennan Schwartz algorithm. The convergence theorems are established when the system matrix is an M-matrix. Numerical experiments show that the proposed methods with alternative direction implicit schemes are efficient and outperform the classical PSOR method and operator splitting method.

Orthogonal Spline Collocation Methods for Space Fractional Diffusion Equation

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Abstract. This paper aims to present orthogonal spline collocation (OSC) method for space fractional diffusion equation. The proposed scheme is based on OSC method for space discretization and finite difference method (FDM) for time. The stability and convergence analysis are rigorously discussed. Last, numerical experiments are carried out to demonstrate the theoretical analysis.

Workshop 2

Computational Mathematics for Oil and Gas Applications

(A workshop in Honor of Prof. Mary F. Wheeler's 75th Birthday)

Invited Talks

An Adaptive Finite Element Method of Two-Phase Flow in Heterogeneous Permeable Media with Different Capillarity Pressures

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Abstract. In this article, we present an adaptive finite element method of two-phase flow in heterogeneous permeable media with different capillarity pressures. Capillary discontinuity may arise from contrast in capillary functions in heterogeneous permeable media, which causes discontinuity in saturation and leads to numerical challenges. In this work, we combine the adaptive mixed finite element and adaptive discontinuous Galerkin methods to solve a consistent formulation in which the total velocity is expressed in terms of wetting-phase potential gradient and the capillary potential gradient. With the help of conforming centroidal Voronoi-Delaunay tessellations, the adaptive meshes are of good quality over a large class of mesh domains even if the grid size varies a lot at any particular refinement level. This helps to overcome the numerical challenges caused by distorted unstructured grids and numerical dispersion effects. Numerical examples demonstrate the efficient and effective implementation of proposed adaptive finite element methods.

An Integrated Solution Program in Shale Gas Play Development and Production

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Abstract. As conventional oil and gas reserves dwindle and oil prices rise, the recovery of unconventional oil and gas (such as heavy oil, oil sands, tight oil/gas, and shale oil/gas) is now the center stage. In particular, the shale gas play development and production will play a significant room in the recovery of unconventional resources. This presentation will be focused

on an integrated solution program in shale gas play development and production in the following areas:

(1) Rich gas regions and "sweet spots" identification and reserve evaluation
(2) Production evaluation and optimization
(3) Well drilling and completion
(4) Formation stimulation

Advanced lab, simulation, well logging and geophysical technologies that support these areas will be addressed. Lab experiments will involve the measurements of petrophysical and petrochemical properties, micro formation structures, and rock mechanics. Simulation will involve the software development of well logs, seismic data, hydraulic fracturing and optimization. Some case studies will be presented. While this presentation is focused on shale gas plays, all the presented lab, simulation, well logging and geophysical technologies also apply to shale oil and tight oil and gas plays.

Modeling Three-Phase Compositional Flow on Complex 3D Unstructured Grids with Higher-Order Finite Element Methods

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Abstract. Most problems of interest in hydrogeology and subsurface energy resources involve complex heterogeneous geological formations. Such domains are most naturally represented in numerical reservoir simulations by unstructured computational grids. Finite element methods are a natural choice to describe fluid flow on unstructured meshes, because the governing equations can be readily discretized for any grid-element geometry. In this work, we consider the challenging problem of fully compositional three-phase flow in 3d unstructured grids, discretized by tetrahedra, prisms, or hexahedra, and compare to simulations on 3D structured grids. We employ a combination of mixed hybrid finite element methods to solve for the pressure and flux fields in a fractional flow formulation, and higher-order discontinuous Galerkin methods for the mass transport equations. These methods are well suited to simulate flow in heterogeneous and fractured reservoirs, because they provide a globally continuous pressure and flux field, while allowing for sharp discontinuities in the phase properties, such as compositions and saturation. The increased accuracy from using higher-order methods improves the modeling of highly non-linear flow, such as gravitational and viscous fingering. We present several numerical examples to study convergence rates and the (lack of) sensitivity to gridding/mesh orientation, and mesh quality. These examples consider gravity depletion, water and gas injection in oil saturated subsurface reservoirs with species exchange between up to three fluid phases. The examples demonstrate the wide applicability of our chosen finite element methods in the study of challenging multiphase flow problems in porous, geometrically complex, subsurface media.

Numerical Methods for Simulating Surface Tension with The Gradient Theory of Fluid Interfaces

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Abstract. The mathematical aspects of the gradient theory for the surface tension of simple fluids and mixtures is rigorously analyzed. The finite element approximation of surface tension is developed and analyzed, and moreover, we present an adaptive finite element method based on a physical-based estimator. An efficient Newton's method for solving the discrete nonlinear equations is developed and analyzed. The numerical tests are carried out both to verify the proposed theory and to demonstrate the efficiency of the proposed method.

Optimal Control Problem of System Governed by Immiscible Displacement Problem in Porous Media

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Abstract. In the field of oil recovery, with the aim to maximize production of oil from petroleum reservoirs, we construct the optimal control problem governed by the modeling system describing the two-phase incompressible flow in porous media in this talk. Then we give the proof for the existence of solutions of our control problem. The optimality conditions are obtained. After that we consider the finite element approximation. Finally, we carry out our numerical simulations.

Droplet Motion with Evaporation and Condensation in One-Component Fluids

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Abstract. Recently, the dynamic van der Waals theory (DvdWT) has been presented for the study of hydrodynamics in one-component fluids with liquid-vapor transition in inhomogeneous temperature fields [Onuki A 2005 Phys. Rev. Lett. 94 054501]. We first derive the hydrodynamic boundary conditions at the fluid-solid interface for the DvdWT using conservation laws and the positive definiteness of entropy production together with the Onsager reciprocal relation. We then apply the DvdWT to the study of droplet motion driven by thermal gradients at solid surfaces. The effect of thermal singularity at the liquid-vapor-solid three phase contact line is investigated. The droplet motion predicted by the continuum hydrodynamic model is also observed and semi-quantitatively verified by performing molecular dynamics simulations for confined one-component two-phase fluids.

An Experimenting Fields Approach to the Numerical Solution of the Navier-Stokes Equations

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Abstract. The numerical solution of the Navier-Stokes equations has always been a challenging task because of its inherent nonlinearity. Furthermore, the set of governing equations do not contain an explicit equation for the pressure which suggests that the continuity equation and the equations of momentum need to be coupled. A few basic approaches exist to dealing with the pressure term either by elimination or by adding an equation for the pressure. Eliminating the pressure may be done by taking the curl of the momentum equation and this produces what is called vorticity equation. In the other approach, an equation for the pressure can be obtained by taking the divergence of the momentum equation to produce Poisson-like equation for the pressure. The third approach is to consider the medium as pseudo compressible and this introduces a time derivative term of the pressure to the continuity equation. The most widely used approach, however, is based on Poisson equation for the pressure. In this approach the numerical algorithm is based on predictor-corrector methods. That is the solution of the momentum equations is first obtained with no pressure gradients, then the solution of the Poisson equation to compute the pressure field at the new time step, then to calculate the final velocity field with the calculated pressure field and ensure the conservation of mass. In this work, we propose another technique in which no need to constructing an explicit equation for the pressure. Rather, all the unknown variables, namely the velocity field and the pressure field are collected in one global system and all are solved at once. Furthermore, the global matrix of coefficients is constructed automatically which makes the discretization simpler and straightforward. This is done by experimenting on the governing equations with a predefined velocity and pressure fields with the outcome are the entries of the global matrix. Although such global matrix is comparatively large compared with that in the previously mentioned approaches, it is more stable in time stepping. Moreover, the fact that the resultant global matrix is largely sparse might be taken advantage of by utilizing a good sparse solver.

Pore-Scale Simulation of Two-Phase Fluid Systems Consisting of Hydrocarbon Components

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Abstract. In this talk, we report our recent work in simulating two-phase fluid systems consisting of hydrocarbon components at a pore scale using a diffusive interface model together with Peng-Robinson Equation Of State (EOS). Peng-Robinson EOS is a widely used realistic EOS for hydrocarbon fluid in petroleum industry, but it imposes a number of challenges in

numerical computation of diffusive interface simulation. In the presentation, we first establish a partial difference equation to model our compositional two-phase system, and we then propose a mixed finite element-based method for the spatial discretization. Splitting and time marching scheme is tricky for the resultant ordinary differential equation system. Most fully implicit methods surprisingly fail to have the desired stability, while a properly-designed semi-implicit time march scheme works very well. This proposed semi-implicit time scheme is based on a convex splitting concept, and it is unconditionally energy stable. The proposed algorithm is able to solve successfully the spatially heterogeneous two-phase systems of hydrocarbon components in two- and three-dimensional domains. We also compare our computational results with laboratory experimental data and verify them with the Young-Laplace equation.

A New Approach to Multi-Phase Field Modeling and Simulation

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Abstract. Phase field models are widely used to describe the two phase system in which each phase is represented by a smooth function called the order parameter. The evolution equation of the system is usually derived by the gradient flow of the total free energy. The generalization of the approach to the N phase ($N \geq 3$) requires some extra consistency conditions in order for the model to give physically relevant results. We propose a projection approach for deriving the evolution equations for the multi-phase system. Efficient numerical methods are also developed for the system. We will also show some numerical results for dynamics of triple junction and four phase contact line.

Numerical Investigations on Turbulent Fluctuations of Additive-Induced Drag-Reducing Flow by Using the Wavelet Decomposition Method

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Abstract. Pipelining is a main manner of oil and gas transportation in the world currently, but many factors like fluctuations of petroleum productivity or marketing variations require adjustable throughput. Adjustment of pipe diameter is not applicable for constructed pipelines. Adjustment of pumping pressure is limited: too low pressure could cause slack flow and cavitation erosion; too high pressure could exceed tolerant pressure of pipelines and cause fracture. To solve this problem, an efficient approach is drag-reducing additives (DRAs) - chemicals which can reduce flow frictions after they are added to the flow. This approach can decrease the designed throughput of pipelines. When a pipeline needs higher throughput, DRAs could be

utilized to promote the throughput at the same pumping pressure by reducing frictions. When a pipeline needs normal or a little lower throughput, DRAs could be canceled. Due to the simplicity and flexibility, DRAs are more and more welcomed by petroleum companies. However, most studies on the mechanisms of drag reduction stay on the statistics, e.g. mean velocity, mean pressure, fluctuation intensity etc. Few studies are made on turbulent fluctuations, which are more complex but more essential characteristics of petroleum pipe flow, so that theory of drag reduction needs improvement to guide the applications of DRAs.

Therefore, in present study, wavelet decomposition method is applied to analyze the multi-scale turbulent structures of drag-reducing flow and heat transfer. Components of velocity fluctuation and temperature fluctuation in different scales are obtained. Effects of DRAs on different scales of flow structures are analyzed. The largest scale of turbulence has lower frequency and larger amplitude. The smaller scales of turbulence appear characteristics of intermittent pulses. These phenomena are quite different from the turbulence without DRAs that almost all scales of motions are irregular high-frequency fluctuations. It indicates that smaller scales of turbulent fluctuations are damped apparently. Further analyzing the energy distribution of all the scales quantitatively, we can find that DRAs mainly change the streamwise fluctuation energy and promote the energy proportion of low-frequency large-scale turbulence from 25% to 80% dramatically. The illustrations obtained from the continuous wavelet transformation show that: DRAs reduce the transitional structures and simplify the turbulent structures so that energy dissipations among different scales are reduced. All of these are inner reasons that DRAs can save energy in turbulent flow. On the other hand, variations of temperature with DRAs are very similar with streamwise velocity. Thus, heat transfer rate is lowered through weaker fluctuations. This is the essential reason of heat transfer reduction.

In all, the wavelet decomposition method can be utilized to reveal or verify multi-scale phenomena of turbulence which are hard to be described or quantitatively explained by conventional methods. It has potential values to guide the flow control of petroleum pipelining. Of course, this method still stays the initial stage for drag-reducing flow and needs improvements in future.

Acknowledgement: This work is supported by National Science Foundation of China (no. 51206186, no. 51174206, no. 51376086) and also by the project entitled "Simulation of Subsurface Geochemical Transport and Carbon Sequestration," funded by the GRP-AEA Program at KAUST.

Modeling Hydraulic Fracturing in Porous Media

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Abstract. We apply a fixed stress splitting for coupling a multipoint flux method for flow in the reservoir with a phase field model for fracture propagation. Computational results showing the robustness of this approach are presented.

This work has been done in collaboration with Andro Mikelic, Gurpeet Singh, and Thomas Wick.

Multiscale Mortar Methods for Multiphysics Applications

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Abstract. We discuss a multiscale framework for multiphysics problems based on mortar domain decomposition methods. The domain is decomposed into a series of subdomains (coarse grid) with different physical processes, mathematical models, and numerical methods. The equations are discretized locally on a fine scale, while interface conditions are imposed weakly on a coarse scale using mortar finite elements. By eliminating the subdomain unknowns, the global problem is reduced to a coarse scale interface problem that is solved efficiently using a multiscale flux basis. Applications to Stokes - Darcy and porous media flow - geomechanics couplings are presented.

Contributed Talks

The Immersed Boundary-Lattice Boltzmann Method for the Simulation of the Flow around Hydrofoils

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Abstract. The flow around hydrofoils is simulated numerically by the immersed boundary-Lattice Boltzmann method (IB-LBM). The lattice Boltzmann method for the simulation of the Navier-Stokes equation is modified by adding a forcing term to account for the no-slip boundary condition. Immersed boundary method is applied to describe effects near non-conducting boundaries in flows. The results of the present study suggest that the proposed IB-LBM methodology provides a powerful numerical tool for simulating the flow around hydrofoils.

An Immersed Interface Method for Solving Two-phase Interfacial Flows

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Abstract. In this talk, an immersed interface method (IIM) for solve incompressible two-phase flows involving interfaces on irregular domains is presented. Two sets of augmented variables are introduced to satisfy the boundary condition for the velocity and the continuity condition of the velocity across the interface. The augmented variables and/or the forces along the interface/boundary are related to the jumps in both pressure and velocity and the jumps in their derivatives across the interface/boundary and applied to the fluid through jump conditions. The resulting augmented equation is a couple system of these two sets of augmented variables, and the direct application of the GMRES is impractical due to larger iterations. In this work, the decoupling of two sets of the augmented variables is proposed, and the decoupled augmented equation is then solved by the LU or the GMRES method. The discretized fluid equations incorporating the jump contributions on a staggered Cartesian grid are solved by the fast solver. The numerical results show that the overall scheme is second order accurate.

An Adaptive NRxx Method for 2D Simulation

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Abstract. Numerical regularized moment method with arbitrary order (NRxx) is able to solve Grad's moment equations or regularized moment equations for arbitrary order of moments. In the present report, the number of order is depend on the local property of the fluid, which provide us an alternative to hybrid method without any artificial layer or inner boundary condition. In the same time, the quality of the mesh grids is guaranteed by a moving mesh strategy. Numerical examples are provided to demonstrate validation and efficiency of the method.

The Compact Difference Method for a Class of Integro-Differential Equations with Completely Monotonic Kernels

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Abstract. A compact difference method is presented for a class of integro-differential equations with completely monotonic kernels. The stability and convergence analysis are proved. Finally, the numerical experiments are given to support the theoretical results.

Workshop 3

Numerical methods for wave propagation

Invited Talks

Fortin Interpolation of Piecewise Non-H1 Space Solution, Edge Element and Adaptive Algorithm of Double Curl Problem with Divergence Free Constraint

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Abstract. A new theory is developed for Fortin interpolation of H(curl)-conforming elements, aiming at very weak solution with piecewise non H1 space regularity in the solution itself and its curl. The non H1 space regularity is typically due to irregular domain boundary and discontinuous anisotropic and inhomogeneous media. When compared with the earlier theory, the significant findings feature several aspects. The Fortin interpolation is suitable for piecewise and very low regular function with non H1 space regularity. The technique is new, with the multiple application of the regular-singular decomposition. Optimal error bounds are established for piecewise non H1 space solutions. Discrete compactness is also shown in the application of the new theory to Maxwell eigenvalue problem. When compared with the so-called co-chain bounded projection, the Fortin interpolation we have developed is suitable for piecewise non H1 space solutions which typically live in discontinuous, anisotropic and inhomogeneous media. Another important advantage is the Fortin interpolation preserves the discrete divergence. These points are not possessed by the co-chain bounded projection.

As an application, we consider the recently developed delta-regularization edge or Nedelec element method with a small parameter delta for the double curl problem with divergence-free constraint. The problem is posed in discontinuous, anisotropic and inhomogeneous media. With the help of the Fortin interpolation, uniform in the parameter delta, optimal error convergence of the resultant finite element solution is shown. A series of numerical experiments are performed to illustrate the theoretical results. In addition, adaptive algorithms are developed. An analysis is carried out and the convergence and the optimality are obtained, uniformly with respect to the parameter delta. Likewise, the Fortin interpolation developed plays a key role in the analysis. Numerical results are presented to confirm the convergence and the optimality of the adaptive algorithm.

Reference

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(2) Huo Yuan Duan, Feng Juan Qiu, Roger C. E. Tan, and Weiying Zheng. *A quasi-optimal convergent adaptive finite element method for the double curl problem with divergence-free constraint*. Submitted to 2013.

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Real-Time Finite Element Solution of Time-Dependent Kohn-Sham Equation

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Abstract. In the authors' previous paper [G. Bao, G. H. Hu, and D. Liu, *An h-adaptive finite element solver for the calculations of the electronic structures*, Journal of Computational Physics, Volume 231, Issue 14, Pages 4967-4979, 2012], a general framework of using adaptive finite element methods to solve the Kohn-Sham equation (KS) has been presented. In this work, we extend this framework to solve the time-dependent Kohn-Sham equation (TDKS). We focus on the real-time methods for TDKS since their potential on handling both linear and nonlinear phenomenon. In this presentation, the background of density functional theory (DFT) and the time-dependent density functional theory (TDDFT) will be introduced briefly. Then both the temporal and spatial discretizations of TDKS, and some numerical techniques on effectively solving TDKS, will be discussed in detail. In particular, an algebraic multi-grid method will be developed for efficiently solving the derived complex-valued symmetric system. Finally, the effectiveness and reliability of our numerical method for TDKS will be demonstrated successfully by a variety of numerical examples for both the linear and nonlinear phenomenon.

A Multi-Level Method for Transmission Eigenvalues of Anisotropic Media

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Abstract. In this talk, we propose a multi-level finite element method for the transmission eigenvalue problem of anisotropic media. The problem is non-standard and non-self-adjoint with important applications in inverse scattering theory. We employ a suitable finite element method to discretize the problem. The resulting generalized matrix eigenvalue problem is large, sparse and non-Hermitian. To compute the smallest real transmission eigenvalue, which is usually an interior eigenvalue, we devise a multi-level method using Arnoldi iteration. At the coarsest mesh, the eigenvalue is obtained using Arnoldi iteration with an adaptive searching technique. This value is used as the initial guess for Arnoldi iteration at the next mesh level. This procedure is

then repeated until the finest mesh level. Numerical examples are presented to show the viability of the method.

Locating Multiscale Ground Objects by A Single Electromagnetic Measurement

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Abstract. In this talk, we consider locating multiple objects on a flat ground by the electromagnetic (EM) measurement made above. The number of the target scatterers might be unknown, and each scatterer could be either an inhomogeneous medium or an impenetrable perfectly conducting (PEC) obstacle. There could also be multiscale components of small-size and regular-size (compared to the detecting wavelength) presented simultaneously. Some a priori information is required on scatterers of regular-size. By using a single EM far-field measurement made above the ground, the proposed method can locate the multiscale scatterers in a very effective and efficient manner.

Near-Field Imaging of Rough Surfaces

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Abstract. Scattering problems are concerned with how an inhomogeneous medium scatters an incident field. These problems have played a fundamental role in diverse scientific areas such as radar and sonar (e.g., submarine detection), geophysical exploration (e.g., oil and gas exploration), and medical imaging (e.g., breast cancer detection).

In this talk, we consider an inverse surface scattering problem in near-field optical imaging, which is to reconstruct the scattering surface with a resolution beyond the diffraction limit. The scattering surface is assumed to be a small and smooth deformation of a plane surface. An analytic solution is derived for the direct scattering problem by using the transformed field expansion, and an explicit reconstruction formula is deduced for the inverse scattering problem. The method works for sound soft, sound hard, and impedance surfaces. It requires only a single incident field with a fixed frequency and is realized efficiently by the fast Fourier transform. Numerical results show that the method is simple, stable, and effective to reconstruct scattering surfaces with subwavelength resolution. Some ongoing and future work will be highlighted along the research line of near-field imaging.

Inverse Elastic Scattering for Multiscale Rigid Bodies with A Single Far-field Measurement

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Abstract. In this talk, we shall describe an inverse elastic scattering scheme for locating multiple rigid obstacles. There might be small obstacles and extended obstacles presented at the same time. The locating scheme is based on some novel imaging functionals. In order to calculate those imaging functionals, only one set of far-field measurement data is required. Moreover, there is no inversion involved in calculating the imaging functionals, and hence the locating scheme is very efficient and robust against noise.

Inverse Scattering Problems: the Effect of Boundary Impedance

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Abstract. For given incident plan waves, the scattered wave outside of an obstacle is governed by the Helmholtz equation in frequency domain. The inverse scattering problems aim to detect the obstacle property such as boundary shape and type from some information about the scattered wave. In the case that the obstacle boundary is of impedance type, the inverse scattering problems need to identify both the boundary shape and the boundary impedance simultaneously . In this talk, we will introduce our recent works for inverse scattering problems of an obstacle with impedance boundary. We will present the reconstruction schemes and show some influence of the impedance distribution on the shape reconstruction performance. Numerical implementations are also given.

Vertical Mode Expansion Method for Some Three-Dimensional Scattering Problems

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Abstract. The mode matching (or eigenmode expansion) method with its many different implementations is widely used for modeling and simulation of scattering and diffraction of electromagnetic waves. Typicaly, one identifies a main propagation direction z, assumes that the structure is piecewise z-independent, and expands the wave field in each z-independent segment in the eigenmodes of the local transverse operator, and calculates the expansion coefficients by imposing proper boundary conditions between the segments. For two-dimensional (2D) structures, the mode matching method is very popular and is often quite accurate. For

three-dimensional (3D) structures, the transverse operator is a differential operator of two transverse variables x and y, the eigenmodes usually can only be calculate numerically. Since many eigenmodes are needed in an accurate implementation of the mode matching method, and they are expensive to calculate, the mode matching method becomes less competitive. We present a different eigenmode expansion method for a class of structures that often appear in application. We assume the structure can be divided into regions where the parameters in each region depend on z only. In each region, we expand the wave field in one-dimensional eigenmodes which are functions of z (the "vertical" modes). The expansion "coefficients" are functions of x and y, they satisfy simple scalar Helmholtz equations. These "coefficients" can be solved by matching the wave fields in different regions. The final linear system is established on the boundaries of the regions, thus the method reduces the original 3D problems to 2D problems.

This is a joint work with Xun Lu and Hualiang Shi.

A Posteriori Error Estimates of Finite Element Approximations of the Incompressible Magnetohydrodynamic Equations

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Abstract. We consider a mixed finite element method for the numerical discretization of a stationary incompressible magnetohydrodynamics problem in three dimensions with its velocity field is discretized using H^1 conforming elements and the magnetic field is approximated by curl-conforming Nédélec elements. Under the assumption that the original model has a unique solution pair, we derive a posteriori error estimates of the incompressible magnetohydrodynamic (MHD) equations with a sharp upper bound. Using these a posteriori error estimates, we construct an adaptive algorithm for computing the solution of 3D magnetohydrodynamics.

This is a joint work with Weiying Zheng.

A GPU-based Recursive Eigen-solver for Transmission Eigenvalues

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Abstract. In this talk, we present an eigen-solver for non-Hermitian eigenvalue problems. The search domain is divided into regular subdomains. The method computes eigenspace projection for randomly generated vectors using contour integrals along the boundary of the subdomain on each GPU core. Then the norm of the projected vector decides whether the contour encloses eigenvalues. The subdomains with eigenvalues inside are further divided smaller subdomains. The procedure is repeated until the size of subdomains is smaller than the required precision. Numerical examples are shown to demonstrate the effectiveness of the method.

Stability Estimates for Multi-wave Inverse Problems

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Abstract. A major problem in solving multi-wave inverse problems is the presence of critical points where the collected data vanishes. The set of these critical points can be identified from the data itself and depends on the choice of the boundary condition. In most existing stability results, the boundary conditions are assumed to be in a small open neighborhood of some CGO solutions where the critical points are controlled. In this talk I will present new stability estimates for some multi-wave inverse problems without assumption on the boundary conditions.

This work has been done in collaboration with Mourad Choulli (University of Lorraine, France).

Fast and Accurate High-order Methods for Wave Scattering Problems

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Abstract. In this talk, we shall present efficient spectral/spectral-element methods for acoustic and electromagnetic wave scattering problems in both frequency- and time-domain computation. To achieve high accuracy, we advocate the use of exact global non-reflecting boundary conditions to truncate the unbounded computational domain, and provide effective analytic-numerical means for computing such artificial boundary conditions (ABCs). We shall also address numerical issues on seamless integration of high-order (bounded domain) and ABCs, and shall consider applications in e.g. cloaking computation.

A Distributional Monte Carlo Method for the Boltzmann Equation

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Abstract. Stochastic particle methods (SPM) for the Boltzmann equation have gained popularity in recent years for the prediction of flows where continuous equations for fluid dynamics are not valid. Among SPMs, the Direct Simulation Monte Carlo (DSMC) methods have been the standard computational method in the field of rarefied gas dynamics. The DSMC method employs a point measure approximation to the distribution function, as simulated particles may possess only a single velocity. This unphysical representation limits the method to converge only weakly to the solution of the Boltzmann equation.

In this talk, we introduce a Distributional Monte Carlo (DMC) method which provides for simulated particles to possess velocity distribution functions, rather than singular velocity vectors. Additionally, we discuss two specific implementations of the technique. The first approach applied kernel density estimation to DSMC. While no variance reduction was observed, the approach was shown to exhibit stronger convergence for the space homogeneous Boltzmann equation. The second implementation represented a hybrid stochastic/deterministic scheme employing the BGK equation for deterministic computation of collision outcomes. When applied to the Bobylev problem, the DMC-BGK method demonstrated a variance reduction of four orders of magnitude over the Nanbu-DSMC method.

Pre-asymptotic Error Analysis of Higher Order FEM and CIP-FEM for the Helmholtz Equation with High Wave Number

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Abstract. In this talk we will show that the pollution errors of p-th order FEM and CIP-FEM in H^1-norm are $O(k^{2p+1}h^{2p})$ under the mesh condition that $k^{2p+1}h^{2p} \leq C_0$ for some constant C_0 independent of the wave number k and the mesh size h.

Variational Methods for the Fluid-Structure Interaction Problem

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Abstract. We are concerned with numerical solutions for the interaction problem of plane acoustic waves in a compressible, inviscid fluid with an elastic structure. The mathematical model can be formulated by a coupling system of the time-harmonic Navier equation in the elastic domain and the Helmholtz equation in the fluid region with appropriate transmission conditions at the interface. We investigate numerical solutions of the problem based on finite element method and boundary integral equation methods. Essential theoretical analysis for numerical models and numerical solutions will be discussed.

This is a joint work with Mr. Tao Yin at CQU, Prof. George C. Hsiao at U of Delaware, and Prof. Joseph E. Pasciak at TAMU.

An FFT-based Algorithm for Efficient Computation of Quasi-periodic Green's Functions for the Helmholtz and Maxwell's Equations

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Abstract. Green's functions are important in the integral equation method for wave propagation and scattering problems. When the medium is periodic in one or two directions, the corresponding Green's functions are quasi-periodic and usually expressed in terms of series. The fast calculation of quasi-periodic Green's functions is usually difficult,in particular, at high frequencies or when a large number of evaluations are needed.

In this talk, we propose an FFT-based algorithm for efficient computation of quasi-periodic Green's functions for the Helmholtz and Maxwell equations in 2D and 3D. Compared with existing algorithms, our algorithm is more efficient at higher frequencies or when a large number of evaluations are needed. The convergence analysis and error estimates are also established. Numerical examples are further provided to illustrate the efficiency of the algorithm.

Optimal Error Estimates for Gaussian Beam Approximation to the Schrodinger Equation

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Abstract. Gaussian beams are generally local asymptotic solutions to the linear wave equations in the high-frequency regime. Each Gaussian beam is concentrated around a specific ray path determined by the underlying Hamiltonian system. Expressed as some superposition of Gaussian beams, Gaussian beam approximation is expected to be a high-frequency asymptotic approximation to the wave function which is globally valid even around caustics. In this talk, we present optimal first order error estimates for Gaussian beam approximations, in both the continuous and the discrete levels, to the Schrödinger equation equipped with a WKB initial data. Our error estimates are valid for any spatial dimension and unaffected by the presence of caustics.

Discontinuous Galerkin Method for Ideal MHD Equations on Tetrahedral Meshes

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Abstract. This talk is focused on the discoutinous Galerkin (DG) method for ideal magnetohydrodynamic equations on unstructured tetrahedral meshes. The DG method is locally divergence-free and preserves the positivity of both the pressure and the density. Numerical experiments will be reported for the simulation of internal kink-modes in toroidal geometry. Parallel scalability will also be shown for large scale simulations.

Contributed Talks

A Dissipation-rate Reserving DG Method for Wave Catching-up Phenomena in a Nonlinearly Elastic Composite Bar

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Abstract. A tensile wave can be destructive, as it can generate microcracks and cause the interface detachments in a composite structure. Recently Huang, Dai, Chen and Kong [Proc. R. Soc. A doi:10.1098/rspa.2012.0292 (2012)] proposed to use material nonlinearity to generate wave catching-up phenomena such that a tensile wave can catch the first transmitted compressive wave, leading to the reduction of the former. They gave the existence and asymptotic solutions in short time. In this paper, we develop a dissipation-rate reserving discontinuous Galerkin (DG) method to solve numerically the system of balance laws with discontinuous flux and inflow boundary condition for waves in a two-material nonlinearly elastic composite bar. Physically, the aim is to examine the reduction ratio of the tensile wave due to wave catching-up phenomena in long time. The stability analysis for the DG method is also presented. And, a contribution is that the numerical fluxes are chosen to satisfy the local dissipation rate across a shock. Numerical results are compared with the available asymptotic solutions in short time and good agreements are found. In particular, the numerical solutions give a high resolution for various interactions between the tensile shock, compressive shock and rarefaction wave. The results confirm that when the stress-strain relation of the second nonlinearly elastic material is convex, indeed the tensile wave can catch the previously transmitted compressive wave. The simulation results by the DG method show that the catching-up phenomena can reduce the magnitude of the tensile wave by more than 400%. We also examine how material parameters influence the reduction ratio. As a verification, the solutions by a WENO finite volume method are also presented, which are in agreement with those by the DG method.

Numerical Simulation and Parameter Identification of One-Dimensional Hyperbolic Telegraph Equation

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Abstract. In this paper, we propose an algorithm for numerical solving the second-order one space-dimensional hyperbolic telegraph equation and identifying the unknown coefficient α, β . The algorithm is based on the Galerkin finite element method and Gauss Newton method in conjunction with the least-squares scheme. The accuracy and efficiency of the procedures are discussed. Some computational results using the newly proposed numerical techniques are presented.

Nonconforming Finite Element Methods for Maxwell's Equations

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Abstract. In this talk, we report nonconforming finite element methods for Maxwell's equations. Generally, the traditional discrete variational formula is not convergent when employing C-R type triangular element since C-R element has been embedded in many FEM softwares. The essential reason is that the piecewise H(div)$\bigcap$H(curl) semi-norm is too weak to control the tangential and normal jumps. Therefore, one way is to employ the interior penalty methods to strong the modified discrete variational formula as well as the nodal vector FEMs for Maxwell's equations. Another is to make use of traditional discrete variational formula by constructing new type nonconforming finite element, in which the piecewise H(div)$\bigcap$H(curl) semi-norm can be controlled by the introduced norm critically. Then, error estimates can run smoothly. Numerical examples demonstrate our theories, too.

A Study of Meshless Local Petrov-Galerkin Method for Scattering by Open Cavities

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Abstract. The study of numerical method of electromagnetic scattering from open cavities has attracted much attention in computational mathematics and electromagnetism because of widely military and civil applications. Many traditional numerical methods, including the method of moments, finite difference, finite element, boundary element and hybrid method have been developed to characterize the scattering from cavities. Unlike the traditional numerical methods, meshless methods greatly reduce the difficulties of generating meshes. Among meshless methods, the meshless local Petrov-Galerkin method (MLPG) was first proposed by Atluri and Zhu for solving linear potential problem, by using domain discretization techniques. The MLPG method is a truly meshless method, which requires no elements or background cells, for either the interpolation or the integration purposes. In the MLPG method, nodal points are randomly spread over the domain of the problem, and the integration of the weak forms is performed on local sub-domains. Therefore no elements or background cells are necessary either for interpolation or integration. In this paper we successfully apply the MLPG to solve the scattering of electromagnetic plane waves by a two-dimensional (2-D) rectangular cavity filled with homogeneous media. Numerical experiments demonstrate the capability of MLPG method for the scattering problem.