Stream 1

Complexity and Approximation in Numerical Analysis

Organizer: Ian Sloan
The Hong Kong Polytechnic University, Hong Kong, University of New South Wales, Australia

Plenary Talk

How to cope with the curse of dimensionality?

H. Woźniakowski
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Abstract. Multivariate problems occur in many applications. They are defined on spaces of functions of d variables and d is often huge. Many of such multivariate problems suffer from the *curse of dimensionality*. This means that the minimal number of functions values needed to compute by algorithms with error at most ε is an exponential function of d. In this talk we discuss how the curse of dimensionality may be vanquished by

- switching to *weighted* spaces where the role of groups of variables is monitored by decaying weights,
- switching to more lenient settings,
- switching to spaces with increasing smoothness of variables.

Study on the numerical methods for TCT image reconstruction

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This talk is based upon joint work with: Shuhuang Xiang (Central South University).

Abstract. We focus on the numerical computation of the integral formulae that are used in Thermoacoustic Computed Tomography(TCT) for image reconstruction. The problem is to numerically approximate these multiple integrals using an series of equi-distribution points in the plane domain. In fact,these integrals involve special functions and typical transforms. First,we solve this problem using Newton-cotes-type formulae. Second,we solve the problem by high-dimensional interpolation and spectral method. The two methods are compared using a diverse range of examples.

$(t, \alpha, \beta, n, m, s)$-nets and $(t, \alpha, \beta, \sigma, s)$-sequences: an overview

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Abstract. In a recent paper [1], $(t, \alpha, \beta, n, m, s)$-nets and $(t, \alpha, \beta, \sigma, s)$-sequences were introduced, which is the topic of this talk. In particular, $(t, \alpha, \beta, n, m, s)$-nets ($(t, \alpha, \beta, \sigma, s)$-sequences) generalize digital $(t, \alpha, \beta, n \times m, s)$-nets (digital $(t, \alpha, \beta, \sigma, s)$-sequences), see e.g. [2], in the same way that (t, m, s)-nets ((t, s)-sequences) generalize digital (t, m, s)-nets (digital (t, s)-sequences).

The talk begins by defining $(t, \alpha, \beta, n, m, s)$-nets. Having introduced $(t, \alpha, \beta, n, m, s)$-nets, one can define $(t, \alpha, \beta, \sigma, s)$-sequences in the same way in which (t, s)-sequences are defined using (t, m, s)-nets.

Subsequently, we discuss some properties of $(t, \alpha, \beta, n, m, s)$-nets and $(t, \alpha, \beta, \sigma, s)$-sequences. In particular, we show that (t, m, s)-nets and digital $(t, \alpha, \beta, n \times m, s)$-nets are special cases of $(t, \alpha, \beta, n, m, s)$-nets ($(t, s)$-sequences and digital $(t, \alpha, \beta, \sigma, s)$-sequences are special cases of $(t, \alpha, \beta, \sigma, s)$-sequences).

A discussion of propagation rules for $(t, \alpha, \beta, n, m, s)$-nets and constructions of $(t, \alpha, \beta, n, m, s)$-nets concludes the talk.

References

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Consistency of Markov chain quasi-Monte Carlo on continuous state spaces

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Abstract. Ordinary Monte Carlo sampling uses independent identically distributed random draws from a distribution, to estimate an expectation. Markov chain Monte Carlo replaces those independent draws by dependent ones and in so doing greatly extends the range of problems that can be addressed. Quasi-Monte Carlo (QMC) replaces random draws by deterministic and equidistributed ones, and for smooth enough integrands, improves accuracy even to the point of improving the rate of convergence. In this talk we present MCMC algorithms which use a completely uniformly distributed sequence as driver sequence and we show that this method consistently gives the correct answer under certain assumptions.

On the complexity of several CME solvers

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Abstract. Systems of chemical reactions involving small numbers of molecules show substantial stochastic behaviour. The probability distributions of these stochastic processes evolve according to the chemical master equations (CME). While the state spaces are discrete, they can be large and even infinite which requires that approximation techniques are used for the solution of the CME. We will in particular consider the characterisation of the chemical reactions by the counts of every single reaction which makes the system into a system of coupled counting processes.

Several approximation methods have been proposed to solve the CME including the stochastic simulation algorithm (SSA), aggregation- disaggregation, finite state approximation, sparse grids, spectral methods, wavelets and perturbation methods. We will discuss the complexity of several of these methods, in particular with respect to the number of reactions. At the end we will explore how graphical models may be used to solve the CME.

Computational issues for kernel-based function approximation

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Abstract. Spline or kriging methods for approximating functions, f, from data are based on symmetric positive definite kernel functions, K. The K serve as reproducing kernels for Hilbert spaces where f reside and facilitate tight worst-case error bounds for approximation. They may also serve as covariance kernels when f is considered to be a stochastic process, and in this case the kernels facilitate average case error bounds. Three important and inter-related computational issues in these kernel-based function approximation methods are: i) determining the sites where the function data is collected, ii) determining the scale and shape parameters that define the kernel from the function data, and iii) efficient computation of the function approximation. This talk discusses recent research in addressing these issues.

PPJD, the parallel scientific package for large sparse polynomial eigenvalue problems

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Abstract. In this talk, we will introduce a newly developed parallel general purpose scientific software package, called the parallel polynomial Jacobi- Davidson (PPJD) package, using two powerful scientific libraries, namely the Portable, Extensible Toolkit for Scientific Computation (PETSc) and the Scalable Library for Eigenvalue Problem Computation (SLEPc) for finding a few eigenvalues of the large-scale polynomial eigenvalue problems (EVP) arising from some discretization of certain partial differential equations in a wide variety of applications in computational science and engineering. PPJD is implemented based mainly on Jacobi-Davidson (JD) algorithm, which is suitable for finding a few interior spectrum of the EVPs. At each JD iteration, one first need to enlarge a search space by adding a new basis vector, which is obtained by solving a large sparse system of equations, known as the correction equations then extract an approximate eigenvalue and eigenvector from the search space through the Rayleigh-Ritz procedure. In the JD algorithm, solving the correction equation is considered to be the most expensive part. Therefore, to design an efficient preconditioner for some iterative method becomes very crucial. Hence we propose a parallel domain-decomposed preconditioner based on the Schwarz framework, which is wildly used and well-understood for solving linear systems, but less studied for solving eigenvalue problems. Our target applications include cubic and quintic polynomial EVPs arising from semiconductor quantum dot simulations. We will present the comparison of the Schwarz preconditioner with other PETSc built-in preconditioners and investigate their parallel performances on a different machines in Taiwan.

Synchronization theory on coupled map lattices with wavelet transform method

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Abstract. The aim of this talk is two-fold. First, we are to give some local synchronization theories [1] of Coupled Map Lattices with general connectivity topology. Second, the theories are then to be used to illustrate the effectiveness of the Wavelet Transform Method for Coupled Map Lattices [2].

References

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A remark on Landau's theorem of lattice point problem and its application to the convergence problem of multiple Fourier series

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Abstract. E. Landau ([1]) proved a estimate of $d(\geq 1)$ dimensional lattice point problem with weights:

$$\sum_{|n|^2<t} e^{2\pi i n x} - \frac{(\pi t)^{d/2}}{\Gamma(\frac{d}{2}+1)}\delta(x) = O(t^{\frac{d}{2}-1+\frac{1}{d+1}}) \quad \text{for all x},$$

where $n = (n_1, n_2, \cdots, n_d) \in Z^d$, $x = (x_1, x_2, \cdots, x_d) \in R^d$, $nx = n_1x_1 + n_2x_2 + \cdots + n_dx_d$, $|n|^2 = n_1^2 + n_2^2 + \cdots + n_d^2$ and $\delta(x) = 1$ if $x \in Z^d$, and $\delta(x) = 0$ if $x \notin Z^d$.

We will prove the following uniform estimation.

Theorem *Let d be any positive integer. We have the following estimation:*

$$\sum_{|n|^2<t} e^{2\pi i n x} - \int_{|\xi|^2<t} e^{2\pi i \xi x} d\xi = O(t^{\frac{d}{2}-1+\frac{1}{d+1}}) \quad \textit{for all } x.$$

Moreover this estimation is applicable to the convergence problem of multiple Fourier series. Let $\chi_a(x)$ be the indicator function of the ball with the center 0 and the radius $a(>0)$ and $f_a(x)$ be the periodization of $\chi_a(x)$, i.e. $f_a(x) = \sum_{n\in Z^d} \chi_a(x+n)$. Then we know that for $d \geq 3$ its Fourier series diverges at $x = 0$(Pinsky, Stanton an Trapa [2]) and for $1 \leq d \leq 4$ converges to $\bar{f}_a(x)$ (the normalization of f_a) at $x \neq$ (Kuratsubo [3]).

Theorem *Suppose $d = 3, 4$, we have the following results.*

$$\lim_{t\to\infty} \sum_{|n|^2<t} \hat{f}_a(n) e^{2\pi i n x} = f_a(x)$$

uniformly in the exterior of any neighborhood of $x = 0$ or $|x| = a$.

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Approximation of the secular function of Rayleigh wave in multilayered medium

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Abstract. The research of the secular function of Rayleigh wave in multilayered medium,is an importment method which can analysis the information of inner stratum.However the complexity and the hidden form of the secular function are an big problems, which limit the inversion work only on theory.This article discusses the approximation of secular function, compares the advantage and shortcoming of different approximation methods on exploration ,such as polynomial approximationsample interpolationtriangle polynomial approximation. Because of the highly oscillatory of the secular function, this paper employs the chebyshev polynomial approximation,and simulates the obvious form of dispersion under the situation of high and low frequency respectively. Through comparison, we find the precision of approximation is high,and the dispersion points are easy to get. Meanwhile,this essay simulates the secular function of complex media, The result shows,the secular function transmits as sinusoidal as the increasing of velocity.The research of this article provide convenience for the geophysical exploration method ,and presents a new thought of studying the dispersion of complex media.

High dimensional model representations in QMC methods for computational finance

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Abstract. The valuation of many financial securities can be formulated as high dimensional integrals for which quasi-Monte Carlo (QMC) methods play an increasing role. This paper investigates the use of high dimensional model representation (HDMR) to improve the performance of QMC methods for high-dimensional problems in finance. Our approaches are based on the low-dimensional approximation for the original multivariate function. To this end, several related problems are studied: (a) the approximation of a function by a sum of lower dimensional functions; (b) the assessment of the possible special properties of high dimensional finance problems, and (c) the effective use of such properties to improve QMC. For problem (a), we prove a new theorem which relates the expected error of the additive approximation to the global sensitivity indices of Sobol'. We also study the problem of how to use a "simple" function to obtain a good approximation. For problem (b), we present a procedure based on HDMR to assess the degree of additivity (a measure of the additive structure) and to generate a good additive approximation. For problem (c), we propose constructive approaches to find a good importance distribution and a good control variate using the additive approximation, and suggest new methods for efficiency improvement, which take the profit of strong additive nature. Numerical examples on high dimensional finance problems illustrate that the proposed methods significantly improve the performance of QMC. Their performance is especially impressive when they are used in conjunction with suitable dimension reduction techniques due to the enhanced additive nature.

Divergence-free kernels and their application to fluid-flow problems

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Abstract. We discuss matrix-valued positive definite kernels in the context of fluid-flow problems. After a short introduction and a review of the basic properties of matrix-valued kernels, we will concentrate particularly on analytically divergence-free approximation spaces generated by such kernels. We will define general approximation schemes for typical fluid-flow problems involving an incompressible fluid. These schemes work in arbitrary space dimension and can produce arbitrary smooth approximations. As typical examples, we will discuss Darcy's problem, the Stokes and the Navier-Stokes equations.

Solving large scale highly nonlinear systems of equations and spherical designs

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Abstract. Spherical L-designs are sets of N points on the unit sphere such that the average of the function values at the points gives the integral over the sphere for any spherical polynomial of degree at most L. Thus they provide the nodes of an equal weight quadrature rule of precision L for the sphere.

Building on a new characterisation of spherical designs by Sloan and Womersley, spherical designs can be characterised by finding a global minimum of zero for an objective function or solving a system of nonlinear equations. This talk concentrates on issues related to solving the resulting large scale (up to degree 100 with 10,000 variables and equations) highly nonlinear system of equations and difficulties with being sure that there is a true solution near to the computed solution.

Error bounds for approximation with Chebyshev points and efficient methods for highly oscillatory functions

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This is a joint work with Xiaojun Chen and Haiyong Wang

Abstract. By using new error estimates for polynomial interpolation in Chebyshev points, we improve error bounds for Gauss, Clenshaw-Curtis and Fejér quadrature and consider their application in generalized Fourier transforms. We show the convergence rates of Chebyshev interpolation polynomials of the first and second kind for numerical evaluation of the integral system involving Bessel or modified Bessel function, which is often more accurate, affordable and much simpler to construct than Levin-type method, and gives error analysis in detail for the Filon-type method with the Chebyshev points. Finally, based on a diffeomorphism transformation, we present an efficient Filon-type method for the integration of systems containing Bessel functions with exotic oscillators, and give applications to Airy transforms. Preliminary numerical results show that the improved error bounds are reasonably sharp.

Fast fourier analysis for high dimensional data

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Abstract. High dimensional data analysis is becoming more and more important in many application areas and is a challenging task. For a d-dimensional function, tensor product type methods will require $O(n^d \log n)$ operations for computing its n Fourier coefficients. When n or d is large, it is extremely difficult to perform the computation if it is not impossible. We present a fast algorithm which requires only $O(n \log^{d-1} n)$ number of operations to compute its n approximate Fourier coefficients. We prove that the approximate Fourier expansion has the same order of convergence as the classical Fourier expansion. Numerical examples will be presented to demonstrate the approximation accuracy and computational efficiency of the proposed method.

A parallel fully implicit solver for the shallow water model on the cubed-sphere

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Abstract. Computer simulations based on the shallow water equations (SWE) play a very important role in many areas of science and engineering including the study of the earth's climate, the understanding of flood, etc. SWE is difficult to solve because its solution admits waves trav- eling at vastly different speeds. To obtain high resolution numerical solutions, supercomputers with large number of processors are necessary. In this work we present a parallel fully implicit solver for the (SWE) on the cubed-sphere. We first present a well-balanced high order finite volume scheme for the SWE in the cubed-sphere curvilinear coordinates, and then discuss a fully implicit time integration scheme in which the time step size is no longer constrained by the CFL condition, which is usually required when using explicit and semi-implicit methods. The price to pay for using a fully implicit method is that a large sparse nonlinear system of equations has to be solved at every time step. We develop and study a parallel Newton-Krylov-Schwarz algorithm to solve the nonlinear system. At each Newton iteration, a linear system is solved using a Krylov subspace method together with a point-block ILU preconditioner. We show by numerical experiments that the algorithm has good accuracy and report the parallel performance of the solver on machines with thousands of processors.

Learning schemes in reproducing kernel Hilbert spaces

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Abstract. Learning theory studies learning function relations or data structures from samples. In this talk I will discuss some learning schemes in reproducing kernel Hilbert spaces for purposes of regression, classification and dimensionality reduction. Some mathematical analysis will be described.

Stream 2

Numerical Solution of Differential Equations

Organizer: Zhong-ci Shi
Academy of Mathematics and Systems Science, China

Plenary Talk

Mathematical modeling in medicine, sports, and technology

Alfio Quarteroni
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and
Politecnico di Milano (Milan, Italy)

Abstract. Mathematical models are enabling advances in increasingly complex areas of engineering, technology and life sciences. Recent developments in mathematical and numerical modeling have opened the way to progress in modeling such complex systems as the human circulatory system, environmental systems and sports for competition. I will talk about this work, and the effort that is made to confront some of the great computational challenges that face us.

Efficient techniques for numerical solutions of some parabolic inverse problems

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Abstract. In this talk we transform a large class of parabolic inverse prob- lem into nonclassical parabolic equation whose coefficients consist of trace type functional of the solution and its derivatives subject to some initial and boundary condition. For this nonclassical problem, we study the finite element approximations, H^1-Galerkin mixed finite element method and the Legendre multi-scaling basis then we present an immediate analysis for superconvergence for these problems.

Emerging applications of spectral methods in quantum and plasma physics

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Abstract. In this talk, I will review different numerical approximations for the nonlinear Schrödinger equation (NLS) in the semiclassical regimes, where the scaled Planck constant is small. I also compare properties preserved in the discretized level of different numerical methods including time reversibility, time transverse invariant, mass conservation, energy conservation, stability, accuracy and resolution in the semiclassical regime. Finally, I show applications of spectral method to different problems in quantum and plasma physics including Zakharov system, Maxwell-Dirac equations and Klein-Gordon Schrödinger equations, etc.

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A robust and accurate finite difference method for a generalized Black-Scholes equation

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Abstract. In this talk, we present a numerical method for a generalized Black-Scholes equation, which is used for option pricing. The method is based on a hybrid finite difference spatial discretization on a piecewise uniform mesh and an implicit time stepping technique. Our hybrid difference scheme used the central difference whenever the local mesh size is small enough to ensure the stability of the scheme; otherwise we use a simple upwind difference scheme. The scheme is stable for arbitrary volatility and arbitrary asset price, and is second-order convergent with respect to the spatial variable. Another distinct feature of our method is that it can handle the degeneracy of the Black-Scholes differential operator at $x = 0$ without truncating the domain. Furthermore, the present paper efficiently treats the singularities of the non-smooth payoff function. Numerical results support the theoretical results.

Optimal grids of least-squares finite element methods in two spatial dimension

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Abstract. This talk concerns a procedure to generate solution-adaptive grid for con- vection dominated problems in two spatial dimensions based on least-squares finite element approximations. The procedure extends a one dimensional equidistribution principle which minimize the interpolation error in some norms. The idea in extending such technique to two spatial dimensions is to select two directions which can reflect the physics of the problems and then apply the one dimensional equidistribution principle to the chosen directions. The final grids generated are then connected through an unstructured grid technique. Model problems considered are the two dimensional convection-diffusion problems where boundary and interior layers occur. Numerical results of model problems illustrating the efficiency of the proposed scheme are presented. In addition, to avoid skewed mesh in the optimal grids generated by the redistribution algorithm, local mesh refinement and smoothing will be considered for suitably weighted least-squares approximations. Comparisons of the solutions with an existing scheme will also be provided.

A greedy algorithm for eigenvalue optimization problems in shape design of two-density inhomogeneous drum

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Abstract. Consider the eigenvalue problem of

$$\begin{aligned} -\Delta u = &\ \lambda\rho(x)u, & x \in &\ \Omega, \\ u = &\ 0, & x \in &\ \partial\Omega, \end{aligned} \tag{0.1}$$

where Ω is a smooth, bounded and connected subset of R^2. Let $S \subset\subset \Omega$ be a sub-domain of Ω. We do not assume any topology on S but its area constrained to a given constant. We assume that the density $\rho(x)$ is a piecewise-constant function

$$\rho(x) = \begin{cases} \rho_1 & \text{for } x \notin S \\ \rho_2 & \text{for } x \in S \end{cases} \tag{0.2}$$

where $\rho_1, \rho_2 > 0$. The eigenvalue optimization problem we need to solve is

$$\max_S \lambda_1 \quad or \quad \min_S \lambda_1 \quad or \quad \max_S (\lambda_2 - \lambda_1), \tag{0.3}$$

subject to the constraint

$$\|S\| = K, \tag{0.4}$$

where $\|S\|$ is the area of S, λ_1, λ_2 are the first two least eigenvalues of (0.1) and K is a prescribed number.

In this paper, we will derive some numerical algorithms for solving the optimization problem (0.3)-(0.4) and present some numerical results.

Fast multilevel augmentation methods for solving Hammerstein equations

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Abstract. Fast multilevel augmentation methods based on projections for solving Hammerstein equations are developed. Each of these methods requires availability of a multilevel decomposition of the solution space and a projection from the solution space onto a finite dimensional subspace. A subspace at a level is obtained from the subspace at the previous level by adding a difference subspace. Accordingly, the projection equation at the present level is obtained by augmenting the projection equation at the previous level. Using this idea recursively, we solve the nonlinear equation (by an iteration method) only at an initial lower resolution level while obtain its solution at a higher resolution level. With the help of the multiscale analysis, we separate the procedure of solving the nonlinear operator equation at a high level into two major components: (1) solving the nonlinear equation only at an initial lower level, and (2) compensating the error by solving a linear system at the high level. We prove that the proposed methods require only linear computational complexity and have the optimal convergence order. A relationship between the proposed method and the multigrid method is discussed. Two specific fast methods based on the Galerkin projection and the collocation projection are developed. Numerical results are presented to confirm the theoretical estimates, with comparisons to the two-grid method.

An interface method based Possoin-Boltzmann equation solver and its application on molecular dynamics

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Abstract. A novel method is presented for solving the Poisson-Boltzmann (PB) equation based on a rigorous treatment of geometric singularities of the dielectric interface and a Green's function formulation of charge singularities. Geometric singularities, such as cusps and self-intersecting surfaces, in the dielectric interfaces are bottleneck in developing highly accurate PB solvers. Based on the matched interface and boundary (MIB) method, we have recently developed an accurate PB solver MIBPB by rigorously enforcing the flux continuity conditions at the dielectric interface where geometric singularities may occur. Meanwhile, in the Green's function formalism, charge singularities are transformed into interface jump conditions, which are treated on an equal footing as the geometric singularities in our MIB framework. This method is able to provide highly accurate electrostatic potentials at a mesh as coarse as 1.2 angstrom for proteins.

An important and direct application of the solution of PBE is to calculate the solvation forces, which are the basis for molecular dynamics (MD) simulation. We provide MIB based solvation forces calculation schemes, taking advantage of the accurate potentials output from MIBPB solver and again the incorporation of interface jump conditions. Accurate reaction field forces are obtained by directly differentiating the electrostatic potential. Dielectric boundary forces are evaluated at the solvent-solute interface using an accurate Cartesian-grid surface integration method. The electrostatic forces located at reentrant surfaces are appropriately assigned to involved atoms. Extensive numerical tests are carried out to validate the accuracy and stability of the present electrostatic force calculation. The present MIB and BP based molecular dynamics simulations of biomolecules are demonstrated in conjugation with the AMBER package.

Optimal Runge-Kutta coefficients for a multi-grid V-cycle

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Joint work with D. Van Heule and J. Vierendeels.

Abstract. Large algebraic systems are primarily solved by iterative procedures. One of the best known is the Runge-Kutta iteration.
We show that the most generally used formulation (e.g. as proposed in [1]) does not allow to form all possible polynomial transmittance functions and we propose a new formulation to remedy this.
Sometimes the Runge-Kutta iteration is used as a smoother for a multi-grid method. In this context optimal coefficients for the Runge-Kutta iteration have been studied in the past (e.g. [2]), which are easily converted to the coefficients used in the new formulation.
The method in which these parameters were established only focuses on the high-frequency content of the error, without taking into account possible interactions with the solver(s) on the coarser grid(s). To investigate this matter, we establish a model for an integrated 2-grid V-cycle [3]; we use this model to find the optimal coefficients for the smoother and compare them with those found in the literature using the advection equation as a model.
It is shown that this optimization approach results in a multi-grid cycle that is up to 33% faster (depending on the type of discretization), even though the smoother in itself is less efficient. It is also shown that a higher number of stages in the Runge-Kutta iteration can result in a better smoother, but that a low number is better when looking at the complete V-cycle.

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The tailored finite point method for singular perturbation problem of second order elliptic equation

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Abstract. In this talk we consider the numerical solutions of singular perturbation problem of second order elliptic equation. When the parameter ε is very small, the solutions of the given problem possess boundary layer and (or) interior layer, this is the essential difficulty for the numerical solutions of singular perturbation problem. We propose a new approach to construct the discrete scheme for the given problem, where our finite point method has been tailored to some particular properties of the solution of the given singular perturbation problem. From our numerical results, we find that the new method given in this talk can achieve very high accuracy with very coarse mesh even for very small parameter ε. In the contrast, the traditional finite element method does not get satisfactory numerical results with the same mesh.

Goal oriented mesh adaptivity for control and state constrained elliptic optimal control problems

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Abstract. We consider adaptive finite element methods for the numerical solution of optimal control problems for second order elliptic boundary value problems with pointwise constraints on the controls and/or the states. The mesh adaptivity is taken care of by an a posteriori error estimator derived by the application of the goal oriented dual weighted approach. The error estimation gives rise to dual weighted residuals, data oscillations, and a primal-dual mismatch in complementarity which can be assessed via the computed finite element approximations. Numerical results are given to illustrate the performance of the suggested approach.
The presented results are based on joint work with Michael Hintermüller.

Convergence of adaptive Morley-type element methods

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Abstract. The adaptive nonconforming Morley-type element methods are developed and analyzed for the 2m-th order elliptic problems. As the substitution of the Galerkinorthogonality property, four important technical results: a discrete efficiency, a quasiorthogonality property, a discrete reliability, and the strict reduction of some total error, are proved. Consequently, the convergence and optimality of these adaptive schemes is established.

On high-order central-upwind schemes for hyperbolic conservation laws

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Abstract. Central-upwind schemes for hyperbolic conservation laws are constructed based on Godunov-typed methods that enjoy the advantages of high resolution, simplicity, universality, and robustness. In this talk, we construct high-order central-upwind schemes obtained by applying convex ENO technique introduced in [2] on the numerical flux of the 2nd order scheme introduced in [1]. The resulted semi-discrete schemes are then solved by an ODE solver. Our high-order central-upwind scheme can be extended to the multi-dimensional case via the rigorous, genuinely multidimensional derivation. Several numerical experiments are performed to show high-resolution and efficiency of our high-order central-upwind schemes.

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A saddle point approach to the computation of harmonic maps

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Abstract. In this paper we consider numerical approximations of a constraint minimization problem, where the object function is a quadratic Dirichlet functional for vector fields and the interior constraint is given by a convex function. The solutions of this problem are usually referred to as harmonic maps. The solution is characterized by a nonlinear saddle point problem, and the corresponding linearized problem is well-posed near strict local minima. The main contribution of the present paper is to establish a corresponding result for a proper finite element discretization in the case of two space dimensions. Iterative schemes of Newton type for the discrete nonlinear saddle point problems are investigated, and mesh independent preconditioners for the iterative methods are proposed.

Multidimensional inverse heat conduction problems

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Abstract. Inverse Heat Conduction Problems (IHCPs) have been extensively studied over the last 50 years. They have numerous applications in many branches of science and technology. The problem consists in determining the temperature and heat flux at inaccessible parts of the boundary of a 2- or 3-dimensional body from corresponding data – called 'Cauchy data' – from

accessible parts of the boundary. It is well-known that IHCPs are illposed which means that small perturbations in the data may cause large errors in the solution.

In this contribution we give an overview over our contributions to multidimensional IHCP's and indicate what computational results for which sort of problems we have obtained. In [1] we have established the theoretical background for multidimensional inverse heat conduction problems. The solutions of the associated direct problem as well as the inverse problem are understood in weak sense (see [1]). This allows the Cauchy data to be only from L_2. The initial condition can be given or not. In the latter case, our method is also able to identify the initial temperature distribution.

The idea of our method is very simple: since the initial condition v_0 and the heat flux $v_1 = \partial u/\partial N|_{S_2}$ at the inaccessible part Γ_2 of the boundary are not known, we consider them as a control $v = (v_0, v_1)$ to minimize the defect $J_0(v) = 1/2\|u(x,\cdot)|_{S_1} - \varphi(\cdot)\|^2_{L_2(S_1)}$ on the accessible part Γ_1 of the boundary. On Γ_0 and Γ_1 different kinds of boundary conditions may be imposed, e.g. homogeneous Neumann boundary conditions on Γ_0 and Dirichlet boundary conditions at Γ_1. The function φ represents the (measured) temperature data on Γ_1. Here, we set $S_i = \Gamma_i \times (0,T], i = 0,1,2$, where $T > 0$ is the final time.

In [1] we have proved the existence of the optimal control, and also obtained the gradient of the defect functional by means of an appropriate adjoint problem. Since the optimal control problem is still unstable, we have to use a regularization method for it.

We solve the underlying inverse problem by discretization in combination with Tikhonov's regularization using a zeroth order penalty term as well as iterative regularization via an appropriate stopping rule. As the underlying operator we choose the Neumann-to-Dirichlet mapping $A : L_2(\Omega) \times L_2(S_2) \longrightarrow L_2(S_1)$ which maps the (unknown) initial function v_0 and the heat flux $v_1 = \partial u/\partial N|S_2$ to $u|_{S_1}$ where u is the solution of the heat equation in weak form. The minimizing functional to determine $v = (v_0, v_1)$,

$$J_\gamma(v) = \frac{1}{2}\left(\|Av - \varphi\|^2_{L_2(S_1)} + \gamma^2\|v\|^2_{L_2(\Omega)\times L_2(S_2)}\right)$$

is differentiable with gradient $J'_\gamma(v) = A^*(Av-\varphi)+\gamma^2 v$ which can be obtained via the solution of an appropriate adjoint problem.

As an iterative algorithm to solve the minimization problem we use the Conjugate Gradient Method (CGM) in connection with an appropriate stopping rule. We allow perturbations of the data, $\|\varphi - \varphi_\varepsilon\|_{L_2(S_1)} = O(\varepsilon)$, and the operator A is replaced by A_h which is a finite element or finite difference approximation.

For the inverse problem calculations we use the *Crank-Nicolson method* for the time integration and the conjugate gradient method plus Tikhonov's regularization to solve the minimization problem described above. The direct solution of the parabolic problems with the Finite Element package DEAL uses bilinear ansatz functions. Our computational results are discussed in detail in [2].

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Two robust C^0 elements with double set parameters for fourth order elliptic singular perturbation problems

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Abstract. The aim of this paper is to present a general convergence theorem of C^0 elements for the fourth order elliptic singular perturbation problems. A new robust C^0 rectangular element and triangular element are constructed with double set parameter method and bubble function technique, and the convergence of new elements are proved in the energy norm uniformly with respect to the perturbation parameter. Numerical experiments are also carried out to demonstrate the efficiency of the new elements.

Convergence analysis for numerical methods to stochastic hyperbolic equations

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Abstract. For a simple model of a scalar wave equation with random wave speed, Gottlieb and Xiu (Commun. Comput. Phys., 3 (2008), pp. 505-518) employed the generalized polynomial chaos (gPC) method and demonstrated that when uncertainty causes the change of characteristic directions, the resulting deterministic system of equations is a symmetric hyperbolic system with both positive and negative eigenvalues. Consequently, a consistent method of imposing the boundary conditions is proposed and its convergence is established under the assumption that the expansion coefficients decay fast asymptotically. In this work, we investigates stochastic collocation methods for the same type of scalar wave equation with random wave speed. It will be demonstrated that the rate of convergence depends on regularity of the solutions, which is determined by the random wave speed and the initial and boundary data. Numerical examples are presented to support the analysis and also to show the sharpness of the assumptions on the random wave speed and the initial and boundary data.

Phase field simulations of two phase fluid flow

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Abstract. In this talk, I will first describe a newly developed phase field model for two phase fluid flow based on Cahn Hilliard Navier Stokes equation with generalized Navier boundary condition. Then some numerical results on two phase flow on rough and patterned surfaces will be presented. Issues related to drop formation, dripping to jetting transition will also be discussed.

Soft-constrained iterative methods for blind source separation

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Abstract. Blind source separation is a statistical inverse problem aiming to recover source signals and mixing filters (discrete Green's functions) without detailed knowledge of the environment. Cocktail party problem is an example of how humans perform this task by paying attention. Yet little is known of the computation inside human brain for this problem. For sound mixtures, source signals viewed as time series are much more independent of each other than their mixtures. The separation is formulated mathematically as minimization of cross correlations. We derive iterative methods from statistical principles, however, the resulting dynamics (differential equations) are nonlinear and solutions may blowup. We devise a class of discrete ordinary differential equations to impose biologically meaningful soft constraints, and control the scaling behavior of iterations. The solutions then exist globally and converge in some weak sense to the desired separation conditions. We also show numerical examples of convergence and sound separation.

Rigorous spectral analysis of optimized Schwarz methods with Robin transmission conditions

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Abstract. In this talk, the tight relationship between Dirichlet-Neumann (D-N) operators and optimized Schwarz methods with Robin transmission conditions is disclosed. We describe the spectral distribution of continuous D-N operators and give a rigorous spectral analysis of discrete D-N operators. By these results, we prove that optimized Schwarz methods with Robin transmission conditions cannot converge geometrically in the case of continuous problems. Furthermore, we get the accurate convergence rate of the two subdomains case. In addition, an estimation of convergence rate of optimized Schwarz methods with Robin transmission conditions is presented in the general case. Most of our results cannot be improved any more.

Relations between the Multiscale Methods for Elliptic Homogenization Problems

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Abstract. In this talk, we will give a short review on multiscale methods for elliptic homogenization problems. We will emphasize the intrinsic links between some popular methods such as generalized finite element methods (GFEM), residual-free bubble methods (RFB), variational multiscale methods (VMS), multiscale finite element methods (MsFEM) and heterogeneous multiscale methods (HMM).

High order PSIC/WENO-Z scheme in shock-particles laden flow

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Abstract. In this talk, I will discuss some recent development and results from the numerical modeling and simulation of dispersal of particle in a supersonic flow by a recently developed high order particle-source-in-cell (PSIC) method. In the high order PSIC method, the Euler equations that govern the gas dynamics are solved with the improved high order weighted essentially non-oscillatory (WENO-Z) scheme. Individual particles (cloud) are traced in the Lagrangian frame using high order Runge-Kutta scheme. A high order interpolation of ENO nature is introduced to determine the carrier phase properties at the particle location in order to avoid interpolation of fluid properties across high gradients in the flow field. A high order central weighting ensures a smooth, low-noise deposition of particle influence on the carrier phase. In the simulation, forty thousand bronze particles packed in the shapes of rectangle, circle and triangle are impulsively accelerated by a Mach 3 shock. In the rectangular shaped particle cloud, particles disperse mostly sideways into material lines that align with the strong shear layers at the side of the cloud in the early time. At the later time, the particle cloud is reshocked by reflected shock from the side channel walls leading to wave patterns along which particles concentrate. We will discuss the effect of the initial particle cloud geometry on the particle dispersion and flow development.

This research is performed in collaboration with Prof. Jacobs at San Diego State University. This work is partially supported by the HKBU Faculty Research Grant for Prof. Don and by the US AFOSR YIP for Prof. Jacobs.

Super-geometric convergence of spectral/spectral collocation methods

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Abstract. Geometric or exponential convergence is one of the most remarkable features of the spectral method. Less well known is the fact that under some ideal situation, the convergence rate of the spectral method and the associated spectral collocation method may exceed the exponential rate. In this talk, we shall discuss such a super-geometric convergence phenomenon in the one-dimensional setting.

Stream 3

Solution Theory and Its Applications in Nonlinear Continuum Mechanics

Organizer: Colin Rogers
The Hong Kong Polytechnic University, Hong Kong
Alex Wai
The Hong Kong Polytechnic University, Hong Kong
K. W. Chow
The University of Hong Kong, Hong Kong

Plenary Talk

Long wave models for internal solitary waves

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Abstract. Large amplitude internal solitary waves are commonly observed in the coastal oceans and atmospheric boundary layer. They can be modeled by evolution equations of the Korteweg-de Vries type, modified to take account of strong nonlinearity and a variable background. We shall sketch the derivation of these models, and then use them to exhibit the propagation and possible disintegration of an internal oceanic solitary wave propagating over the continental slope.

Extreme solitons: dangerous or useful ?

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Abstract. The family of soliton equations is enormous. Started with the KdV equation, the soliton theory made a remarkable progress in the field of integrable equations. Nonlinear Schrödinger equation was the second in a row of being solved using the inverse scattering technique. Among many others, its solutions help us to tackle an intriguing problem of rogue waves in the ocean. These can be called "waves that appear from nowhere and disappear without a trace" (WANDT) [1]. There is a hierarchy of these solutions with increasing order and with progressively increasing amplitude. These waves can appear from smooth initial conditions and they can have virtually infinite amplitude. The final stage of evolution is their complete disappearance.

The presence of dissipation plays a crucial role in the soliton dynamics. To balance loss, the system has to have a continuous energy supply from a larger reservoir. In these conditions the system may have infinite number of fixed soliton solutions. The best example is the complex cubic-quintic Ginzburg-Landau equation (CGLE) which is basically a modified nonlinear Schrödinger equation. The set of the localized states described by the CGLE is far from being completely classified and it is unlikely that it ever be. We are faced with the necessity to study myriads of types of solitons and countless number of bifurcations between them. One of the many fascinating features of these solitons is the increasing amount of soliton energy at certain region of the system parameters. The phenomenon can be called "dissipative soliton resonance". These solutions have variety of applications in physics, mechanics and optics. In particular, they describe generation of record high-energy pulses by laser oscillators [2].

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Solitons in optical communications

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Abstract. Soliton solutions of the nonlinear Schrodinger equation have been a key concept in high speed optical communications since 1980. Their particle like nature has often been useful as a conceptual hook on which to base a deeper understanding of system performance. Key properties such as stability to perturbations, self-similarity, global attractors and phase coherence have been applied. In this talk I will discuss some of these properties of solitons in both a systems context and in their application to laser physics and to optical switching. Finally some of the recent work of the Aston group will be covered.

Modulation instabilities and periodic patterns in systems of coupled nonlinear Schrödinger equations

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Abstract. Systems of coupled nonlinear Schrödinger equations (NLSEs) occur in a variety of physical contexts, e.g. multiple wave guides in optical fibers and mode interactions in stratified fluids. Here the modulation instabilities (MI) of plane / continuous wave and some special exact, periodic solutions of such coupled systems are studied:

(1) MI can occur in coupled NLSEs if the magnitude of the cross phase modulation (XPM) is larger than that of the self phase modulation (SPM), even if each mode is in the stable regime if isolated individually. While this feature has been proven in optics, the first contribution here will be a demonstration of this fact for waves in fluid.

(2) Sets of coherently coupled NLSEs will arise in the polarization of light beams or the quartet interactions of gravity waves in hydrodynamics. The distinguished feature of these systems is that the relative phase of each individual waveguide now plays a crucial role in the dynamics, as opposed to the well studied classical models like the Manakov equations. Peculiar features of these coherently coupled NLSEs studied include:

(a) The full MI equations will be treated without making any approximations usually invoked earlier in the literature, in particular, birefringence effects will be permitted to be nonzero.

(b) The role of cross phase modulations will be investigated.

(c) Double humped solitary pulses will be derived analytically. Their stability will be studied numerically by the split step Fourier methods.

Electromagnetic field simulation of corrugated surface-wave discharges

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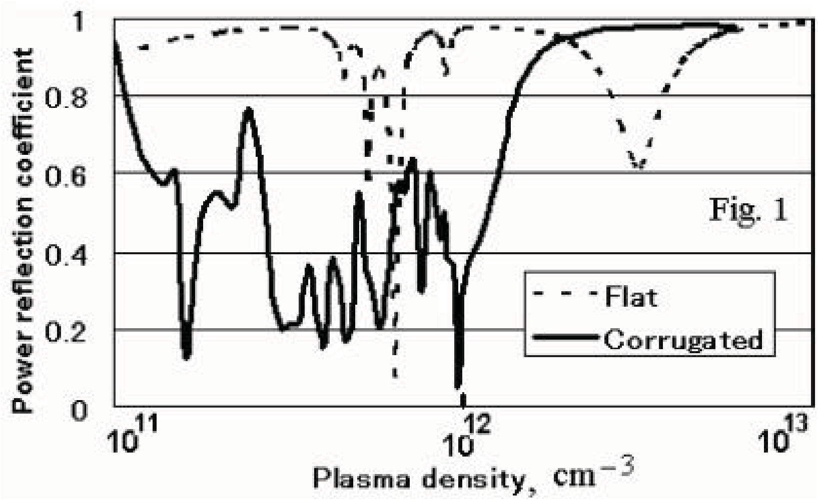
Abstract. Surface electromagnetic waves propagating along the interface between high-density plasma and a dielectric medium are known to sustain stable and clean discharges, which have found wide application to industrial plasma processing, in particular i n the manufacturing of advanced semiconductor devices. Since high-density plasmas can be penetrated by microwaves only up to the depth of the thin skin layer, devices located further away from the plasma-dielectric interface are protected from direct microwave damage. The absence of electrostatic coupling ensures low plasma potential, reducing the risk of damage by high-energy ions. Recently, much interest has been generated by the effects of corrugations and hollows along the dielectric wall facing the plasma in such surface-wave discharges. Corrugations and hollows have been shown [1, 2] to (A) reduce or eliminate mode jumps; (B) allow stable discharge operation at much lower power levels; (C) improve the plasma uniformity; and (D) increase significantly the average plasma density. Various explanations have been proposed, but the phenomenon is not well understood yet. In past works [3] we have shown that corrugations modify the dispersion of the surface waves travelling along the corrugated interface, which tentatively explains some (A and B) of the observations. In the present contribution we present

a numerical study of a more realistic case: a finite cylindrical discharge chamber with a corrugated dielectric (quartz) plate of finite thickness as the top wall. The microwave is launched by a radial slot antenna fed by a coaxial cable centered along the cylinder axis. The corrugations are chosen to be axially symmetric too (coaxial rings centered at the chamber axis), which ensures an ideal axiallysymmetric geometry suitable for two-dimensional numerical analysis. After solving numerically Maxwell equations in such a model for a series of realistic plasma densities, we deduce the microwave power reflection coefficient at the reference plane on the entrance of the coaxial cable. The results are shown in Fig. 1,



compared to the case of a classical surface-wave discharge with flat non-corrugated plasma-dielectric interface. Flat-interface surface-wave discharges are known to reflect almost all incident electromagnetic power, except at a few specific resonant plasma densities, as shown by the dashed curve in Fig. 1. This is an obstacle to the operation at low power: one needs enough power to reach at least the lowest resonance density. Moreover, increasing the incident power further does not lead to a smooth increase of plasma density. Instead, at first only the reflected power increases, until the power gets high enough to achieve a jump (called "mode jump") to the next higher resonance density. The solid curve in Fig. 1 explains why corrugations mitigate this behavior: First, significant power absorption becomes possible at much lower densities, thus lowering the threshold for discharge ignition, and, second, high absorption is achievable over a much wider density range, eliminating the wide density jumps when varying the power. The numerical simulation procedure described above has potential for optimizing the corrugation geometry and excitation conditions. Experimental data confirming this behavior will be presented, too.

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New geometric polyhedral models for nanotubes

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Abstract. The conventional model for carbon nanotubes [1] imagines that a graphene sheet is rolled into a cylinder, with the tacit assumption that atoms and bonds in the flat plane can be curved around the idealized surface of a cylinder. This model is useful when the effects of curvature are minimal. However, for the smallest radii nanotubes, the effect of curvature becomes significant and cannot be neglected. In order to capture the essential consequences of curvature, we develop a new polyhedral model [2, 3] based on three fundamental principles: (i) all bond lengths are equal; (ii) all bond angles are equal; and, (iii) all atoms are equidistant from the cylindrical axis. From these assumptions alone, we derive an exact model constructed from triangles, and generate explicit relations between the chiral vector numbers (n,m) and the geometric quantities such as the radius, unit length and bond angle. An asymptotic analysis of the new model shows that, to leading order, the new expressions agree with the conventional formulae. A new formula is produced for the corrugation in the tube wall, which can be thought of as the nanotube "thickness." The predictions of the new model are compared with several ab initio computational studies and excellent agreement is found. The model is extended to boron nitride nanotubes [4] where the two atom species adopt two different cylindrical radii in the one nanotube. In this case the principle of bond angle equality must be modified and we assume that the bond angles in the more rigidly bonded species (i.e. boron) maintain an equiangular configuration, but the other bond angles are allowed to vary. From this modified principle a more general model is developed which is shown to agree well with ab initio calculations in the literature. Further, we present a number of related new results arising from corresponding geometric models of nanotubes for boron and silicon, and including models with distinct bond lengths and distinct bond angles.

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Two discrete integrable systems and their applications

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Abstract. In the first part of my talk, a q-difference version of the ϵ- algorithm is proposed, which may be viewed as the q-difference version of the modified Toda molecule equation. It is shown that this algorithm can be used to compute the approximation $\lim_{t\to\infty} f(t)$. In the second part of the talk, motivated by recent work of Fukuda A,Ishiwata E,Iwasaki M and Nakamura Y (Inverse Problems **25**(2009) 015007), we design another new algorithm for computing eigenvalues of a given matrix from a generalized form of the discrete Lotka-Volterra (gdLV) system.

This is joint work with Y. He, J.Q. Sun and H.W. Tam

Energy localization and solitons in nonlinear periodic systems

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Abstract. I will overview the recent achievements in the study of the energy localization and solitons in a variety of nonlinear systems where the effects of discreteness and periodicity become important. This is planned as a panoramic overview of several fields that will cover, in particular, (i) generation and control of optical gap solitons in waveguide arrays and photonic lattices, including the recent observation of polychromatic gap solitons generated by a supercontinuum source, (ii) localized matter waves of Bose-Einstein condensates in two- and three-dimensional optical lattices, (iii) discrete localized magnetic states in composite metamaterials, and (iv) energy localization and transport in carbon nanotubes.

First of all, I will emphasize the most important recent advances in nonlinear optics where many of novel theoretical findings have been verified in experiment. This includes the observation of surface solitons in one- and two-dimensional photonic lattices, the observation of polychromatic "rainbow" gap solitons in photonic lattices generated by a supercontinuum source [1], the generation of topologically stable spatially localized multivortex solitons, etc.

One of the recent concepts in the theory of nonlinear waves is associated with a novel type of broad nonlinear states which appear in the gaps of the bandgap spectra of periodic systems such as light waves in periodic photonic lattices and Bose-Einstein condensates in optical lattices. These localized states cannot be treated by familiar multi-scale asymptotic expansion techniques, and they can be better understood as truncated nonlinear Bloch waves [2]. I will demonstrate that these self-trapped localized nonlinear modes can be found in one-, two-, and three-dimensional periodic potentials, and they have been readily observed in experiments on nonlinear self-trapping of matter waves in one-dimensional optical lattices.

Finally, I will discuss the energy localization in carbon nanotubes and demonstrate the existence of spatially localized nonlinear modes in the form of discrete breathers [3]. In nanotubes with the chirality index $(m, 0)$ there exist three types of discrete breathers associated with longitudinal, radial, and torsion anharmonic vibrations, however only *twisting breathers* survive in a curved geometry remaining long-lived modes even in the presence of thermal fluctuations.

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Solutions of the reaction-diffusion system related to the resonant nonlinear Schrödinger equation

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This is a joint work with O.K. Pashaev.

Abstract. At first, we will review some old results about 2 by 2 AKNS system and the related evolution equations and the solution methods.Then we will make a brief report on the resonant nonlinear Schrödinger equations and reation-diffusion systems and the application[1], [2]. A novel integrable version of the NLS equation namely [1],

$$i\frac{\partial\psi}{\partial t}+\frac{\partial^2\psi}{\partial x^2}+\frac{\Lambda}{4}|\psi|^2\psi=s\frac{1}{|\psi|}\frac{\partial^2|\psi|}{\partial x^2}\psi.$$

has been termed the *resonant nonlinear Schrödinger equation* (RNLS). It can be regarded as a third version of the NLS, intermediate between the defocusing and focusing cases. The critical value $s = 1$ separates two distinct regions of behaviour. Thus, for $s < 1$ the model is reducible to the conventional NLS, (focusing for $\Lambda > 0$ and defocusing for $\Lambda < 0$). However, for $s > 1$ it is not reducible to the usual NLS, but rather to a reaction-diffusion system, which can be transform into Kaup-Broer system. In this case, the model exhibits novel solitonic phenomena [1].

The RNLS can be interpreted as an NLS-type equation with an additional 'quantum potential' $U_Q = |\psi|_{xx}/|\psi|$. Very recently it was shown that RNLS naturally appears in a reduced equation in the plasma physics[3].

A Hirota bilinear representation of the Reation-Diffusion system with non-zero boundary condition is given.Here some exact solutions are obtained by Hirota bilinear method. Recently we notice that the derivative Reaction-Diffusion system can be transformed into Reaction-Diffusion system.So in this sense,DNLS with 'quantum potential' is related NLS with 'quantum potential' . Recently we also consider generalized nonlineat Schrödinger equation in this direction.

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Quick inversion of Rayleigh wave fundamental mode dispersion curves in a multilayered medium in which velocities increase monotonically

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Abstract. Rayleigh wave is a kind of surface wave which has dispersion character in layered medium. Utilizing this, Rayleigh wave inversion method is more and more used in geophysical prospecting, ultrasound nondestructive detection and so on in recent years. There are many kinds of Rayleigh wave inversion method. However, most of them are time taking. Here a method that much quicker than others is presented. It has been proved that the Rayleigh wave dispersion function is a kind of linear transformation T with respect to S-wave velocity of each layer when the velocity of the medium increases monotonically. Made use of this character, we gave out a quick inversion method of Rayleigh wave fundamental mode dispersion curves. In this method, corresponding to n different wavelengths, we can find an $n \times n$ matrix U. Then, once n dispersion points of these n wavelengths (whose phase velocity can form an n-dimensional vector A) are obtained from measured signal, $U \times A$ is just the S-wave velocity of each layer we want to know. Here the matrix U is obtained from the dispersion curves correspond to n given models whose S-wave velocity vectors are linear independent.How to give the n models such that U is available is discussed.Finally, inversion of given multilayered medium with this method shown that the precision is acceptable.

Multiple vortex interaction models: symmetries, conservation laws and vortex sources

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Abstract. Many vortices might exist simultaneously for a complex fluid system. In this report, some possible multiple vortex interaction models are established. The symmetries and conservation laws of the models are studied. It is found that the momenta, vortex momenta and the energies of every one vortex and the interaction energies of every two vortices are conserved. For the idea fluid, some special types of exact vortex source solutions including multiple point vortices, vortex dipoles, vortex multi-poles, fractal cyclons and fractal cyclon dipoles are presented. For the rotating fluids, to get exact explicit multiple vortex source solutions, additional flow-flow interactions are introduced.

Dynamical symmetry breaking in dual-core nonlinear systems

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Abstract. Fundamental models of various physical media based on configurations with two parallel cores (waveguides) amount to systems of linearly coupled equations. The simplest example is the model of dual-core optical fibers or planar waveguides, which amounts a system of coupled nonlinear Schrödinger (NLS) equations for amplitudes of electromagnetic waves in the two cores [1],

$$\begin{aligned} iu_z + (1/2)u_{\tau\tau} + |u|^2 u + v = 0, \\ iv_z + (1/2)v_{\tau\tau} + |v|^2 v + u = 0. \end{aligned} \tag{1}$$

An obvious symmetric soliton solution to this system, with $u = v$, loses its stability through a *symmetry-breaking bifurcation* (SBB) of the *subcritical* type, when its energy exceeds a certain critical value. The SBB simultaneously gives rise to stable asymmetric solitons. SBBs accounting for the transition between symmetric and asymmetric solitons were studied in detail too in a number of other models. Some of these models also originate in nonlinear optics, describing dual-core fiber Bragg gratings with the intrinsic Kerr nonlinearity [2], linearly coupled waveguides with the quadratic [3] or cubic-quintic [4] nonlinearities, or a set of two parallel discrete waveguide arrays [5] (in the latter case, the SBB predicts the transition between discrete symmetric and asymmetric solitons). In addition to that, a number of works treated the SBB in models of Bose-Einstein condensates confined to a set of two parallel "cigar-shaped" traps, coupled by tunneling of atoms [6, 7]. Generic features of the SBB are that it happens with symmetric solitons in models with the self-focusing intra-core nonlinearity, and with antisymmetric solitons in the case when the nonlinearity is self-defocusing, which is most typical to BEC settings. In the latter case, the localized states featuring the bifurcation are actually *gap solitons* [2, 7], and the SBB is a bifurcation of the *supercritical* type, in contrast to that in system (1). While a majority of the studies of the SBB were dealing with one-dimensional (1D) models, a 2D model for the BEC trapped in two parallel "pancake"-shaped field configurations was studied too [8]. Actually, the nonlinearity can give rise to SBB not only in models supporting solitons, but also in other settings, a recent example being the bifurcation studied in a 1D model with a double-well *pseudopotential,* i.e., a nonlinear potential, described by the following equation [9]:

$$iu_t + (1/2)u_{xx} + [\delta(x-a) + \delta(x+a)]\,|u|^2\,u = 0.$$

All the above-mentioned models describe conservative media. The SBB was also studied in dissipative nonlinear models, *viz.*, in a system of two linearly coupled complex Ginzburg-Landau equations with the cubic-quintic nonlinearity [10]. In that case, the bifurcation happens to solitary pulses ("*dissipative solitons*").

The presentation will aim to give an overview of basic models, results, and physical applications of the symmetry-breaking phenomena in conservative and dissipative nonlinear media.

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Darboux transformations on time scales

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Abstract. A times scale is an arbitrary closed subset of the real numbers, possibly containing both continuous and discrete components. Studying dynamics on time scales gives a unified approach to continuous, discrete and q-discrete models and new models on mixed-type domains. We will consider some examples of integrable systems on time scales and show that a generalized Darboux transformation may be used to construct solutions in a more or less standard way. Other applications of these generalized Darboux transformations, for example to supersymmetric systems, will be discussed briefly.

The envelope soliton resonances: basic ideas and new results

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Abstract. Integrable Hamiltonian perturbations of the generic envelope soliton equations are considered. With complex-valued field of the soliton, two motions, the center-of-mass motion and internal oscillations in the envelope, are characterized by corresponding velocities. Inspired by analytical mechanics in generalized coordinates, we choose kinetic energy of the fluid motion to be determined in terms of pseudo-Riemannian metric as a generic quadratic form in the generalized velocities. It produces dispersion terms for the envelope field as the standard dispersion, the quantum potential and the Malomed-Stenflo type forms. Diagonalization of the quadratic form for positive definite metric corresponds to the standard dispersion, while for the degenerate metric the model is reducible to the corresponding dispersionless limit. We show that the negative signature metric produces the quantum potential modification of the model and develops causal singularity of black hole type. In this case the integrals of motion allow the fusion and fission of solitons and interaction of solitons shows the resonant character. We illustrate the general idea by several examples. In 0+1 dimensions nonlinear doubled damped oscillator with hyperbolic symmetry is considered. In 1+1 dimensions: the resonant nonlinear Schr?dinger equation (RNLS), which appeared first in description of black holes in Jackiw-Teitelboim gravity and the theory of constant curvature surfaces in pseudo-Euclidean space. It governs also the transmission of uni-axial waves in a cold collisionless plasma, subject to a transverse magnetic field. Resonant DNLS and modified DNLS as descriptive of the chiral soliton resonances related with one dimensional anyons are discussed. Resonances in generalized NLS by Malomed-Stenflo would be considered. Two and three resonant soliton interactions with web-like structure in Resonant Yajima-Oikawa and the Resonant Long-Short wave interaction systems would be present. Integrable hierarchy of the resonant soliton equations in 1+1 dimensions and generated by it soliton resonances for KP-II and MKP-II in 2+1 dimensions would be discussed.

On shell membranes, the Lame equation and Enneper surfaces

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Abstract. We demonstrate how the classical Lame equation arises out of an integrable system of equilibrium equations for shell membranes. In the simplest case, we thereby obtain particular families of parallel Enneper surfaces as viable membrane geometries.

Wu's mass postulate and solutions of the fKdV equation

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Abstract. Wu's remarkable finding of upstream-advancing solitons in water flows over a topography revived the nonlinear wave research in the 1980s. Wu and his colleagues numerically and experimentally found that a transicritical water flow over bump generates a train of upstream-advancing solitons, a depression zone at the downstream of the topography, and a wave zone further downstream. Wu attributed this intriguing phenomenon to the solutions of several mathematical models, including the forced Kortweg-de Vries (fKdV) equation. Wu (1987) postulated that the excess mass of the upstream-advancing solitons comes almost entirely from the region of surface depression (pp.81-82). With this postulate, the depth of the downstream depression zone can be found from the solvability condition of a boundary value problem of an ordinary differential equation. Further, when the topography base is relatively short compared to its height, the depression's depth can be explicitly written as a function of the upstream flow speed and the topography's cross-section area but not the shape. Then from Wu's theorem of mass, momentum and energy, the approximate solutions of the fKdV equation can be found. The epsilon-invariant theorem and infinitely many choices of epsilon values will be discussed when using fKdV as an asymptotic approximation model. The meaningful size of epsilon is in the range of 0.4-0.7, excluding values close to zero (Shen, 1992). Numerical simulations of collision of soliton-twins and stability of stationary solutions together with the satellite observations of the upstream-advancing solitons in the atmosphere over Hainan Island, China will be presented (Zheng et al., 2004).

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L-isothermic surfaces

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(based on joint work with Colin Rogers and Wolfgang Schief)

Abstract. It has recently been shown that a class of L-isothermic surfaces arises naturally out of a classical system of equilibrium equations for shell membranes. It is demonstrated that these surfaces can be generated via a non-homogeneous linear differential equation of second order. Such description of the L-isothermic surfaces proves useful for analyzing Bäcklund transformation. The Bäcklund transformation for generalised Dupin cyclides will be presented.

Stream 4

Applications of Engineering Mathematics

Organizer: C. K. Chan
The Hong Kong Polytechnic University, Hong Kong
Man-Kam Kwong
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Plenary Talk

Advances in advancing interfaces: efficient algorithms for inkjet plotters, semiconductors, medical scanners, and seismic imaging

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Abstract. Propagating interfaces occur in a wide variety of settings, and include ocean waves, burning flames, and material boundaries. Less obvious boundaries are equally important, and include iso-intensity contours in images, handwritten characters, and shapes against boundaries. In addition, some static problems can be recast as advancing fronts, including robotic navigation and finding shortest paths on contorted su rfaces.

One way to frame moving interfaces is to recast them as solutions to fixed domain Eulerian partial differential equations, and this has led to a collection of PDE-based techniques, including level set methods, fast marching methods, and ordered upwind methods. These techniques easily accommodate merging boundaries and the delicate 3D physics of interface motion. In many settings, they been proven valuable.

The talk is an overview of these approaches, with an eye towards fundamental mathematical ideas and their geometric and algorithmic interpretation. Applications will be framed around industrial engineering collaborations which have led to robust codes for semiconductor manufacturing, inkjet plotters for building plasma displays, image segmentation and tracking in cardiac scanners, robotic navigation, and seismic imaging in oil recovery.

On the univalence of functions with logharmonic Laplacien

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Abstract. In this paper, we prove Radó's theorem holds for functions of the form $F(z) = r^2L(z)$, L is logharmonic. We show that if F is of the form $F(z) = r^2L(z)$, $|z| < 1$, where $L(z) = h(z)\overline{g(z)}$ is logharmonic, then F is starlike iff $\psi(z) = h(z)/g(z)$ is starlike. In addition, when $F(z) = r^2L(z) + H(z)$, $|z| < 1$, where L is logharmonic and H is harmonic, we give the sufficient conditions for F to be locally univalent.

On the dynamics of mixing of a thermally stratified shear layer

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Abstract. Recently, there has been much interest in applying methods from dynamical systems to the study of transport and mixing in fluids. For example, in 2-D time periodic flows, the transport dynamics can be reduced to the study of the associated Poincaré map on R^2. In such flows the mechanism for chaotic transport is the existence of hyperbolic fixed points for the map and the transverse intersection of their associated invariant manifolds.

In other cases, the mixing region can be characterized using the Okubo-Wiess criteria which is based on considering the evolution equation of the velocity gradient in the limit of the vanishing vorticity in a Lagrangian invariant under the assumption that vorticity and strain are solely varying with respect to the vorticity gradient in a Lagrangian frame.

Further information on particles convection is provided by the study of absolute and relative dispersion: Absolute dispersion (also called particle dispersion) provides a measure of the mean square displacement of individual particles at time t, while relative dispersion is defined as the mean square displacement at time t between a pair of initially nearby particles.

The other tool used to describe the "good" mixing is the correlation function$H(r)$ which is the number of pairs of points in the mixing domain whose separation is less than r. The slope of the log-log graph of $H(r)$ gives the fractal dimension (the correlation dimension) ν of the attractor. In the plane, for example, a "good mixing" or complete mixing will occur when ν is close to 2.

In this article, a survey of the above mentioned tools and some of the most recent mathematical tools used to describe the fluids mixing will be presented.

Effect of velocity slip on Newtonian fluid flow in an eccentric annulus

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Abstract. Solution of a large number of problems in modern technology involves flow in pipes whose cross sections are doubly connected regions. This study has its importance, whenever simultaneous flow of two fluids has to be considered. The flow of a Newtonian fluid in an eccentric catheterized artery is studied analytically and a closed form solution is obtained. The arterial segment is assumed to be straight, arterial wall is rigid and permeable and the flow is fully developed. A Newtonian fluid flowing in an annular domain D the $x - y$ plane bounded internally by a circle C_1 and externally by a circle C_2. The method involves mapping eccentric circles in $x - y$ plane onto concentric circles in $\xi - \eta$ plane, using conformal mapping. The mapping $z = \frac{c}{1-\zeta}$ where $z = x + iy$, $\zeta = \xi + i\beta$, transforms conformally the ring space enclosed by two eccentric circles to a region enclosed by two concentric circles with radius ρ_1 and ρ_2 with $\rho_1 < \rho_2$. The boundary conditions for the above problem are given by no-slip velocity on the boundaries C_1 and BJ slip condition on C_2. The solution for velocity distribution and rate of flow are obtained in the closed form and graphically plotted for different values of eccentricity and permeability. The important parameters that govern the rate of flow are the eccentricity of annulus and permeability parameter. The eccentricity of the annulus facilitates transport of more fluid than concentric annulus. The permeability parameter reduces the rate of flow due to loss of fluid.

Computation on interface capturing in a complex geometry

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Abstract. Interface capturing in a complex geometry works in a wide range of applications, such as exhausted gas bubbles of high explosive underwater. In this paper, we extend GFM method to a three dimensional arbitrary curvilinear coordinate system. Eulerian equations are discretized by upwind TVD scheme to describe flow field, and level-set equations by 5th WENO scheme to obtain bubbles' evolution. Level-set equation and extrapolated variables equation are also coordinate transformed. The computations are conducted in parallel and multi-block approach. Boundary information is communicated based on MPI. We simulate expansion of a high pressurized gas bubble initially underwater and also conduct a computation the expansion of V-shape high-pressurized gas bubble in a cylinder. The domain is divided into 5 blocks. The results demonstrate extension of GFM, in this paper, to a complex geometry is capable of capturing interfaces with high ratios of pressure and density underwater.

A quenching criterion for multi-dimensional parabolic problems due to a concentrated nonlinear source

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Abstract. A criterion for the quenching of the solution for a one-dimensional semilinear parabolic first initial-boundary value problem with a concentrated nonlinear source situated at b is given. The locations of b for global existence of the solution and for the quenching of the solution are given. A correct formulation of the problem in multi-dimensions is discussed, and a quenching criterion is given.

Quenching for nonlinear degenerate parabolic problems

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Abstract. For the problem given by $u_\tau = \left(\xi^r u^m u_\xi\right)_\xi / \xi^r + f(u)$ for $0 < \xi < a$, $0 < \tau < \Lambda \leq \infty$, $u(\xi, 0) = u_0(\xi)$ for $0 \leq \xi \leq a$, and $u(0, \tau) = 0 = u(a, \tau)$ for $0 < \tau < \Lambda$, where r is a nonnegative constant less than 1, a and m are positive constants, $f(u)$ is a positive function such that $\lim_{u \to c^-} f(u) = \infty$ for some positive constant c, $u_0(x)$ is a given function satisfying $u_0(0) = 0 = u_0(a)$, this paper studies the quenching of the solution u.

Capturing of free surface in flow impacting walls from a broken dam

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Abstract. Although Marker and Cell(MAC) was firstly proposed in 1965, there is a revival of the MAC method since 1990s. GENSMAC code can deal with generalized Newtonian flow both two and three dimensions. Anyway, MAC method is still robust for tacking interface characterized by large deformation during fluid impacting on walls in flood disaster. This is typical interaction between incompressible Newtonian or non-Newtonian fluid and structure. In this paper, we extend MAC method to three dimensional curvilinear frame in complex geometry. Fully Navier-Stokes equations are solved in staggered grids in transformed frame to obtain flow pressure and velocity field. Meanwhile, virtual particles(markers) are set in cells in transformed domain and their positions are updated according to the latest computed velocity field. MAC method was used to track the free surface with large deformation during fluid impacting walls. Based on MPI and multi-block methods, paralleled computations were conducted to obtain the flow-field and evolution of free surface. The pressure contours, flow velocity and free surface depicted by makers can be obtained in the computation. By pressure histories on wall surface, the stress and strain solution can be either got by solving solid equations in Lagarangian frame with finite element method(FEM). Then, we can know the stress distribution and deformation of walls. These information are valuable in evaluating safety of concrete structure. The results show that free surface with large deformation can be effectively captured by MAC method and its extension is capable of dealing with complex geometry. This method has potential application in safety evaluation of structure especially in the case of flood disaster.

Large eddy simulation on coherent structures in rectangular methane non-premixed flame

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Abstract. Large eddy simulation of a three-dimensional spatially developing transitional free methane non-premixed flame is performed. The solver of the governing equations is based upon a projection method. The Smagorinsky model is utilized for the turbulent subgrid scale terms. A global reaction mechanism is applied for the simulation of methane/air combustion. The simulation result clearly illustrates the coherent structure of the rectangular non-premixed flame, consisting of three distinct zones in the near field. The periodic characteristic of coherent structures in the rectangular non-premixed flame is discussed. The predicted structure of the flame is in good agreement with the experimental result. The distributions of species concentrations across the flame surfaces are illustrated, and typical flame structures in the far field are analyzed. Local mass fraction analysis and flow visualization indicate that black spots of the flames are due to strong entrainment of oxygen into the central jet by streamwise vortices, and breaking up of the flame is caused by enormous entrainment of streamwise vortices and stretch of spanwise vortices at the bottom of the flame.

Some exact blow-up solutions to Euler-Poisson equations and an unique exact solution to an initial value problem of Liouville equation

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Abstract. In this paper, we will present an exact unique solution to an very important initial value problem (IVP) of Liouville's equation. By this result, we successfully construct some exact solutions to Euler-Poisson equation, some of which are unsteady and compressible, some of which is steady and incompressible. What's more, the two unsteady solution to Euler-Poisson equation will blow up in finite time at the origin. These result partly solve two open problem regarding astrophysics and differential geometry. Up to now, to Euler-Poisson Equations, this is the first time to successfully construct exact solution. This significant success has partly pave the road to the global analysis of the global behavior of Euler-Poisson Equation in astrophysics.

The valid range of thin timoshenko beam theory based on finite element method

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Abstract. The solution of the Timoshenko beam theory (TBT) leads to two kinds of flexural waves, first spectrum (TBT1) and second spectrum (TBT2). These two spectrums are also called s_a-wave and s_b- wave respectively. Direct computational simulation based on the finite element method (FEM) was carried out to detect the valid range of the solution in a thin Timoshenko beam. The results show the valid range for s_a-wave should be higher than some reference reported and the upper limitation can increase to double of the critical frequency, at least for simple supported beams. On the other hand, there is no clew from the results to support the existence of s_b-wave. The disagreement aspects of the TBT and the FEM result are maybe caused by the shear coefficient used in the TBT governing equations.

The secret of flight by computation

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Abstract. We show by computational solution of the incompressible Navier-Stokes equations with friction force boundary conditions, that the classical inviscid circulation theory by Kutta-Zhukovsky for lift of a wing and laminar viscous boundary layer theory by Prandtl for drag, which have dominated 20th century flight mechanics, do not correctly describe the real turbulent airflow around a wing. We show that lift and drag essentially originate from a turbulent wake of counter-rotating rolls of low-pressure streamwise vorticity generated by a certain instability mechanism of potential flow at rear separation. We use a stabilized finite element method with duality-based a posteriori error control, which allows computational prediction of the flight characteristics of an airplane using millions of meshpoints without resolving thin boundary layers, instead of the imposssible quadrillions required according to state-of-the-art for boundary layer resolution.

We present applications to the flight of an airplane, helicopter, paraglider, bird, boomerang, frisbee, discus, and to sailing, swimming and paddling, as well as spin in ball sports, and the action of a propeller and wind turbin, [4, 1]. The new theory of lift and drag is a consequence of the recently published resolution of d'Alembert's paradox [2, 3] and a new theory for separation in slightly viscous flow [5].

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Nonlinear p-Laplacian problems with various types of singular weights

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Abstract. In this talk, several existence results of positive solutions for one-dimensional weighted p-Laplacian problems will be presented. In particular, with three types of singular weights, variation of existence, non-existence and multiplicity of solutions due to different singular effects as well as boundary conditions will be discussed. The talk is mainly based on the following reference.

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Two time-splitting numerical methods the Maxwell-Dirac system

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Abstract. Two time-splitting numerical methods are presented for solving the Maxwell–Dirac systems. One is a time-splitting spectral method, which is based on a time-splitting discretization of the Dirac equations, and then approximating nonlinear equations by pesudospectral method for spatial derivatives and solving the ordinary differential equations (ODEs) in phase space analytically. It is explicit, unconditionally stable, conservative, and of spectral-order accuracy in space and second-order accuracy in time. Another is a time-splitting difference method, in which the Maxwell equations with particle and current densities as the source terms are discretized explicitly. The Dirac equations coupled electromagnetic potentials are discretized by the time-splitting method and implicit finite difference. This difference method is conservative and has second-order accuracy in time and space. It can deal with simulation of the Maxwell-Dirac system with singular conditions. Several examples are given to test the accuracy, describe dynamical behaviors of the system with special external potentials and compare two methods.

Computation of quasi-periodic phononic crystals band gaps basing on nonhomogeneous second-order ODEs

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Abstract. Lumped-Mass (LM) method is widely used to solving the periodic phononic crystals and gaps, but for non-periodic phononic crystals it doesn't work. In this article, we deduce a simplified vibration equation for non-periodic crystals based on the main idea of LM method. Then, the problem of computation of the band gap of non-periodic crystals can be seen as solving a nonhomogeneous second-order ODEs. Based on the characters of the nonhomogeneous second-order ODEs and the solutions, we present an improved Lumped-Mass (ILM) method for the computation of the quasi- or non- periodic phononic crystals band gaps. Compared with the finite difference method, ILM method is much more efficient and more useful to understand the physical natures of phononic crystals.

Computation on fluid-structure interaction in a confined volume

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Abstract. In petroleum engineering, exhausted gas of powders with high temperature and pressure is often used to enlarge perforation in rocks. This is a typical problem of flow structure interaction (FSI) related to impact loading. We adopt a piecewise parabolic method (PPM) solving the Arbitrary Lagrangian Eulerian (ALE) equations to flow field solution issued from charged powder. Finite element method (FEM) is used to solve virtual work equations in Lagrangian frame to get rock dynamic responses. Failure criterion is used to determine damaged rock based on magnitude of stress or strain. Pressure and normal velocity are reset on the interface between fluid and solid. Time step of solid computation is referred as entire computation because of high sound speed. Complex geometry is cut into multi-blocks and boundary information is based on MPI model. The computation is paralleled to increase efficiency. In this paper, distributions of pressure are presented to show that shock waves generate inside the cylinder and propagate both inside the cylinder and perforation in the rock. Von Mises stress contours are also presented to illustrate the mechanism.

A two-phase sub-grid-scale kinetic energy model for large eddy simulation of dense gas-solid flows

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Abstract. In present two-fluid large-eddy simulation of gas-solid flows, the same form of Smagorinsky sub-grid-scale (SGS) model for both two phases is adopted, and for dense gas-particle flows, it is combined with the particle kinetic theory as a LES-2p-SM- model. In such a treatment, the interaction between two phases in the sub-grid scale is not taken into account. A gas-particle two-phase kinetic energy SGS model together with the particle kinetic theory is proposed as a LES-K-Kp- model. Both two models are used to simulate dense gas-particle flows in a riser. The results show that the particle concentration and velocity obtained using the first model agree well with the experimental data and are much better than those obtained using the second model. Furthermore, the results show core-annulus flow structure. The anisotropic features of particle dispersion and normal Reynolds stress of particle fluctuation in axial direction larger than those in radial direction are illustrated. The dominant frequency value is equal to 0.27 by the power spectrum analysis of particle concentration. Keywords: kinetic energy SGS mode ; dense gas-particle flow; LES; Riser

Approximation property of T-S fuzzy singular systems

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Abstract. This article focuses on the approximation problem of T-S fuzzy singular systems, the approximation theorem of T-S fuzzy singular systems is proposed. It demonstrates that T-S fuzzy singular systems could approximate a wide class of nonlinear singular systems to arbitrary accuracy. And, the MISO(multi-input single-output) situation is extended to MIMO(multi-input multi-output) situation, which exists more wildly and the nonlinear singular systems are MIMO systems essentially. Based on this approximation theorem and using Neural Network method, the model of T-S fuzzy singular systems could be constructed. The structure and learning algorithm are given later. In this paper, two Neural Network training strategies are proposed and their advantages and disadvantages are analyzed respectively. Finally, a numerical example is given to illustrate the validity of the algorithms.

Elastically restrained orthotropic shallow spherical shells with imperfections under a concentrated load

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Abstract. This paper deals with non-linear behaviors of an imperfect orthotropic shallow spherical shell continuously supported on a non-linear elastic foundation under a concentrated load at the center. Based on the asymptotic iteration method (AIM), an asymptotic solution is derived, and the cubic analytical relation between the external load and central transverse displacement (deflection) of the shell in the form of non-dimension is given. The resulting relation incorporates the effects of geometrical imperfection factor, edge-restraint coefficients, moduli of foundation, characteristic geometrical parameter and orthotropic parameter, and can be adopted readily to evaluate the effects of these factors on deformation and buckling behaviors of the shell structure. Numerical examples are demonstrated and compared with the available results for some special cases. The results show that the asymptotic solution is proven to have enough exactness in computation.

Large eddy simulation of premixed combustion under varying swirl numbers

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Abstract. Using a wide-spread finite volume code for solving the low-pass filtered Navier-Stokes equations, OpenFOAM, the author(s) investigate flow and flame for a lean premixed swirl stabilized flame while varying the swirl number. The burner is also investigated experimentally to provide a validation of the numerical results. The design idea is very simple; the swirl number may be changed by partly injecting the fuel/air mixture tangentially into a pipe. The current design allows for a swirl number ranging from zero up to about 3. The flame is found at the exit of the burner, and is dynamically stabilizied in the diverging flow field. The flow is modeled using large eddy simulation, LES, and combustion is modelled using a single-step reaction with a partially stirred reactor model, PaSR. While varying the swirl number different flame shapes are obtained. At low swirl numbers the flame blows off, while flashback is observed at higher swirl numbers ($S \sim 1.5$). At low swirl numbers the flame is lifted off the burner with a rather flat flame base. As the swirl number is increased a conical flame base forms and propages upstream, approaching flashback.

3D elasticity analysis of laminated cylindrical shell with piezoelectric layer

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Abstract. Piezoelectric materials have been widely used as distributed sensors and actuators in the area of smart structures for the purpose of active structural control. On the other hand, the lightweight high-strength laminated shells with piezoelectric layers have found extensive applications. Hence, the behavior of these structures under mechanical and electrical loadings has been studied. In this research, an elasticity solution is developed for the analysis of coupled Electrical-Mechanical problem in a simply-supported, orthotropic, layered piezoelectric cylindrical shell with finite length under dynamic load. The cylindrical shell is subjected to axisymmetric load. The highly coupled partial differential equations (p.d.e.) are reduced to ordinary differential equations (o.d.e.) with variable coefficients by means of trigonometric function expansion in longitudinal direction for displacement and external forces. The resulting ordinary differential equations are solved by Galerkin finite element method and suitable time marching scheme. Numerical examples are presented for [0/90/P] lamination with sensor and actuator for different thicknesses.

Mathematical modeling and computation for moisture transport in fibrous materials

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Abstract. Mass and heat transfer in fibrous porous media can be found in numerous industrial and engineering applications such as textile, paper and pulp, building materials and more recently in the electrodes of proton exchange membrane fuel cells. In these applications, modeling becomes increasingly important as it provides an efficient and cost effective way for evaluating new designs or testing new materials. In this talk, we present our recent work on moisture transport model in fibrous clothing assemblies in a one dimensional setting. We formulate this problem as multi-phase flows in fibrous porous media with phase change. The model is based on a previous study with significant modification to take into account the air resistance to moisture transport as well as the capillary effect on liquid water motion. An efficient semi-implicit numerical scheme is proposed for solving the gas (vapor and air) and energy equations while the water equations are solved separately. Our numerical solution agrees well with the quasi-steady approximate solution. Qualitative comparison between the numerical results and the experimental measurements are also given.

Numerical study of statistical temporal scales in inertia-particle dispersion

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Abstract. Statistical temporal scales revolved in inertia-particle dispersion are analyzed numerically. The numerical method of large eddy simulation, solving a filtered Navier-Stokes equation, is utilized to calculate fully-developed turbulent channel flows with Reynolds number of 180 and 640, and Lagrangian trajectory method is employed to track the inertia particles released into the flow fields. The Lagrangian and Eulerian statistical temporal scales as a function of distance from the channel wall are obtained for fluid-tracer particles and three kinds of inertia particles with Stokes number of 1, 10 and 100 respectively. The Lagrangian temporal scales increase from the wall to the channel central plane while the Eulerian temporal scales of fluid-phase decrease, and shorter than the Lagrangian ones. The inertia particles Lagrangian temporal scales increase with particle Stokes number. Due to particle inertia and particle trajectory crossing effects, the Lagrangian temporal scales of fluid-phase as seen by particles, obtained by integrating the velocity correlation functions, are separate from those of fluid-phase obtained by tracing the fluid-tracer particles. Reynolds number effects on the integral temporal scales are also presented.

Study on extraction method of dispersion curve by generalized S-transform

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Abstract. In this paper we present a new method for extraction of dispersion curve from multi-channel Rayleigh wave by S-transform. Although several time-frequency analysis methods have been used to extract dispersion curve, the defects of time-frequency window make some information of dispersion curve missing or wrong. S-transform is an extension of the ideas of CWT, and is based on a moving and scalable localizing Gaussian window. It have some desirable characteristics that are absent in the STFT and CWT. The same to the WVD, it can provide time-frequency joint function, but doesn't have cross terms. It's an time-frequency analysis method that has superior performance. So in this paper, we use generalized S-transform to extract dispersion curve, and propose the method of using the slope of the straight line that fitted by extreme points of multi-channel Rayleigh wave to estimate group velocities. We analyze the signal form two-layer medium of containing soft underlying layer and three-layer medium of containing soft interlayer by the new method, and compare results with the dispersion curves that get by scalar-transfer algorithm, the error is less than 10%; Use our method to analyze the measured Rayleigh wave signal, and compare the result with the dispersion curve getting by STFT method, it's more smooth and can reflect the underground structure accurately. That provides reliable basis for inversion interpretation in Rayleigh wave exploration.

Large-eddy simulation of an ethylene-air turbulent premixed V-flame

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Abstract. Large-eddy simulation using a dynamic eddy-viscosity sub-grid scale stress model and a fast-chemistry combustion model without accounting for the finite-rate chemical kinetics is applied to study the ignition and propagation of a turbulent premixed V-flame. A progress variable c-equation is applied to describe the flame front propagation. The equations are solved two-dimensionally by a projection-based fractional step method for low-Mach number flows. The turbulent inflow is produced by mesh grid generated turbulence. The flow field with a stabilizing rod without reaction is first obtained as the initial field and ignition happens just upstream of the stabilizing rod, and the shape of the flame is affected by the vortex structure. Following the flame propagation, the vortices fade and move along the flame front. The LES computed time-averaged flame angle and time-averaged velocity agree well with data obtained from experiments.

Large eddy simulation of gas-particle swirling flow using subgrid-scale second-order moment two-phase turbulent model

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Abstract. The research focal point of gas-particle turbulent flow is to construct a rational subgrid-scale (SGS) closure model of particle phase turbulent flow under the framework of Euler-Euler two-fluid model using large eddy simulation method (LES). A new gas-particle subgrid-scale second-order moment two-phase turbulent model is established, and an algebraic expression of two-phase turbulent kinetic energy correlation is presented to reflect interaction between gas and particle by the method of dimensional analysis. Meanwhile, gas particle-particle temperature two-vortex viscosity model (GP-θ-SGS), taking account of the effects of small scale particle fluctuation for particles collision is built up based on the formalization of gas turbulent flow SGS model and the theory granular dynamics. These models are used to close and solve the SGS Reynolds stress and turbulent viscosity of gas-particle two-phase two-fluid turbulent model. By using them, numerical simulation is carried out for gas-particle flow in coaxial-jet combustor. Results showed distribution of the particle concentration and the particle velocity agreed well with experimental data. Furthermore, predicted results of particle and gas phase fluctuation velocities are superior to Reynolds-averaged simulation methods.

A soft computing algorithm for disassembly sequencing

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Abstract. In recent years, it is an important issue to handle products at the end-of-life (EOL). In order to efficiently recover the EOL products, it is necessary to disassemble the product into several smaller components in this process. However, the disassembly time is dependent on the disassembly sequence of components. The purpose of the study is to obtain the optimal disassembly sequence of the product which can minimize the disassembly time. In this paper, we propose a soft computing algorithm to solve this problem by combining modified discrete particle swarm optimization (DPSO) with concept of precedence preservative crossover (PPX) in genetic algorithm. Discrete particle swarm optimization is a population based stochastic optimization technique, and PPX guarantees feasible solution at each of evaluations. Finally, a benchmark problem shows the efficiency of this approach.

Numerical simulation of internal flow-field of a swirl coaxial injector in a hot environment

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Abstract. Based on the fractional volume of fluid (VOF), a pure Eulerian model for defining and capturing the gas/liquid interface is developed in this paper. This model can define gas/liquid interface in high refinement and is better than the original VOF methodology. To validate the proposed model and the algorithm, a computational code is employed to predict the flow performance in a cylindrical swirl injector under cold-flow condition. Simulated results agree well with experimental measurements. Furthermore, the proposed model is used to simulate gas-liquid reacting flows inside a gas/liquid coaxial swirl injector operating in a hot-fire environment. The turbulent combustion process is simulated with the k--f-g model. Numerical simulation is carried out under actual operating condition of the coaxial injector. Injector performance such as liquid film thickness, liquid film injection velocity, spray angle, and pressure drop are obtained based on detailed information of the internal flowfield. Simulated results also show that droplets are shed from the liquid film in the recess cup of the coaxial injector due to the large velocity gradient between the gas and the liquid streams with a burning area, characterized by high temperature, present inside the injector.

A V-cycle multigrid method for a viscoelastic fluid flow satisfying an oldroyd-B-type constitutive equation

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Abstract. A V-cycle multigrid method is developed for a time-dependent viscoelastic fluid flow satisfying an Oldroyd-B-type constitutive equation in two-dimensional domains. Also existence, uniqueness, and error estimates of an approximate solution are discussed. The approximate stress, velocity, and pressure are, respectively, σ_k-discontinuous, u_k-continuous, and p_k-continuous.

Traveling waves of non-local reaction diffusion equations

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Abstract. In this talk I will talk about traveling waves to delayed reaction diffusion equations. It includes three parts, and the first part is about the background of wave propagation. I will present the Fisher equation, traveling waves for the Fisher equation and other standard reaction diffusion equations. Simulations are provided to show the real solution patterns. In the second part, we study a non-local reaction diffusion model. I will show how to derive the non-local term, why we have the non-local term inside and how to study the traveling wave patterns. We will concentrate on two cases: monostable and bistable. In part three, we apply our non-local reaction diffusion system to study a disease transmission model. Here we present a case study of rabies in Europe.

Size effect of deformation in beams, plates and shells

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Abstract. Experimental results have shown that the bending of beams is influenced significantly by the thickness when the thickness is reduced to the order of the characteristic length of the beam materials. It is so called size effect. Size effect issue arises always in the micro structures since the characteristic length of metals generally is several microns. In order to model the size effect an improved theory of beams, as well as an improved theory of plates and shells are developed. The approach is based on the strain gradient - dependent elasticity. The presented theory indicates that the bending rigidity of beams, plates and shells is dependent on the ratio of the characteristic length of materials and the thickness of the structures. This dependence describes the size effect.

Thermally coupled Quasi-Newtonian flows: analysis and computation

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Abstract. In this paper, we consider an incompressible quasi-Newtonian ow with a temperature de- pendent viscosity obeying a power law, and the thermal balance includes viscous heating. The corresponding mathematical model can be written as:

$$\begin{cases} -2\nabla\cdot(\mu(\theta)|D(u)|^{r-2}D(u))+\nabla p &= f & \text{in} & \Omega \\ \nabla\cdot u &= 0 & \text{in} & \Omega \\ -\triangle\theta &= \mu(\theta)|D(u)|^{r} & \text{in} & \Omega \\ u &= 0 & \text{on} & \Gamma \\ \theta &= 0 & \text{on} & \Gamma \end{cases}$$

where $u:\Omega\to R^d$ is the velocity, $p:\Omega\to R$ is the pressure, $\theta:\Omega\to R$ is the temperature, Ω is a bounded open subset of R^d, $d=2$ or 3, Γ is boundary. The viscosity μ is a function of θ, $\mu=\mu(\theta)$. $D(u)=\frac{1}{2}(\nabla u+\nabla u^T)$ is the strain rate tensor, and $1<r<\infty$. Some mathematical results such as existence and uniqueness are established, finite element approximation is proposed, and convergence analysis is presented.

A high order accurate upwind compact finite difference scheme with group velocity control for shallow water equations

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Abstract. In this paper we investigated an upwind compact finite difference scheme with group velocity control for better simulation of shallow water equations.Compared with traditional difference schemes, compact schemes have higher accuracy for the same stencil width. In order to suppress numerical oscillations,the group velocity control technique is combined with the upwind compact scheme to solve the shallow water equations.A splitting method is also used to deal with the source terms in shallow water equations.Numerical solutions indicate that the method is satisfactory.

Stream 5

Computational Optimization

Organizer: Liqun Qi
The Hong Kong Polytechnic University, Hong Kong

Plenary Talk

A unified framework for dynamic pari-mutuel information market design

Yinyu Ye
Stanford Universtiy

Abstract. Recently, several new pari-mutuel mechanisms have been introduced to organize markets for contingent claims. Hanson introduced a market maker derived from the logarithmic scoring rule, and later Chen & Pennock developed a cost function formulation for the market maker. On the other hand, the SCPM model of Peters et al. is based on ideas from a call auction setting using a convex optimization model. In this work, we develop a unified framework that bridges these seemingly unrelated models for centrally organizing contingent claim markets. The framework, developed as a generalization of the SCPM, will support many desirable properties such as proper scoring, truthful bidding (in a myopic sense), efficient computation, and guarantees on worst case loss. In fact, our unified framework will allow us to express various proper scoring rules, existing or new, from classical utility functions in a convex optimization problem representing the market organizer. Additionally, we utilize concepts from duality to show that the market model is equivalent to a risk minimization problem where a convex risk measure is employed. This will allow us to more clearly understand the differences in the risk attitudes adopted by various mechanisms, and particularly deepen our intuition about popular mechanisms like Hanson's market-maker. In aggregate, we believe this work advances our understanding of the objectives that the market organizer is optimizing in popular pari-mutuel mechanisms by recasting them into one unified framework.

Sensitivity analysis in obstacle problems

J.F. Bonnans
Ecole Polytechnique

Abstract. We will apply general tools of sensitivity analysis for optimization problems in a Banach space setting, to the study of static displacements in continuum mechanics in the presence of obstacles. We will discuss three examples of a beam, a membrane filled with liquid, and a clamped plate.

1. J.F. Bonnans, A. Hermant: Stability and Sensitivity Analysis for Optimal Control Problems with a First-order State Constraint. ESAIM:COCV 14-4(2008), 825-863.

2. J.F. Bonnans, C. Pozzolini: Sensitivity analysis in obstacle problems for a beam and a plate. INRIA Report, in progress.

3. R. Bessi Fourati, J.F. Bonnans, H. Smaoui: The obstacle problem for water tanks. J. Math. Pures et Appliquées 82-11(2003), 1527-1553.

A novel approach in multilinear least-squares with application to design of filter networks

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Joint work with Mats Andersson, Hans Knutsson, Bjorn Svensson

Abstract. Filter networks is a rapidly developing area due to their ability to significantly lower the computation time in multidimensional signal processing, especially in medical imaging. The design is based on solving a multilinear least-squares (MLLS) problem where the use of conventional methods is often practically impossible, because it is a non-convex large-scale optimization problem with a lot of local minimizers. The existing approaches are characterized by a lack of robustness - a very slow convergence with no guarantee of success. They are typically based on generating random initial points for further refinement with the use of local search methods.

So far, successful network designs have been restricted to special types of filters, e.g. those used for analyzing local signal structures. The lack of efficient methods for solving MLLS is however a bottleneck for further progress in filter network design.

Our approach is based on a reformulation of the MLLS problem in the form of a new optimization problem which allows us to deal with the multi-extremal nature of the original problem. Its solution is used then as an initial point in the original MLLS problem for further refinement.

We present results of numerical experiments which testify to the efficiency and robustness of our approach. Comparing to the standard approach, it demonstrated a speedup factor of several hundred in designing sub-filter sequences for 2D low-pass, band-pass and high-pass filters.

A generalized Fischer-Burmeister merit function for the second-order cone complementarity problem

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Abstract. In this talk, we will introduce a new merit function ψ_p for the second-order cone complementarity problem (SOCCP), which includes the popular Fischer-Burmeister (FB) merit function as a special case. The class of merit functions was well studied for the nonlinear complementarity problem (NCP) and shown to possess all favorable properties as the FB merit function holds. We will show that the generalized FB merit function is differentiable when $p \in (1, 4)$, and furthermore, it is continuously differentiable when $p \in (1, 2]$. Then, we provide a mild condition to guarantee that the generalized FB merit function has bounded level sets. Numerical results will be also reported to illustrate the influence of the parameter p on the performance of the merit function approach based on the unconstrained minimization of the generalized FB merit function with $p \in (1, 4)$.

General scenario tree generation algorithms under GARCH models

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Abstract. The quality of multi-stage stochastic optimization models depends heavily on the quality of the underlying scenario tree model to describe the uncertain environment. The existing scenario generation algorithms are improved from the following aspects: to properly reflect variations in higher order moments of the underlying random data process, we propose a new simulation approach for the scenario generation under GARCH models; to improve the current sequential optimization scenario generation method, the GARCH model is used to recursively estimate central moments of the stochastic data process needed in the sequential scenario generation process, and a new hybrid intelligent algorithm is designed to solve non-convex programming problems encountered during the sequential optimization process, derived from which is an efficient new-type sequential optimization method for general multistage scenario tree generation under multivariate GARCH models; finally, numerical results with trading data from Chinese stock markets illustrate the efficiency, flexibility and practicality of our algorithms.

Polynomial interior point methods for $P_*(\kappa)$ nonlinear complementarity problems

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Abstract. Primal-dual interior point methods(IPMs) are the most efficient methods for both computational and theoretical points of view. But there is still a gap between the practical behavior and the theoretical complexity result of large-update IPMs. Peng et al. proposed new variants of IPMs based on self-regular barrier functions and improved the complexity result up to $O(\sqrt{n}\log n \log \frac{n}{\epsilon})$ which is so far the best known complexity result for such methods. And they generalized to second order cone optimization(SOCO) and semidefinite optimization(SDO). Recently, Roos et al. proposed new primal dual IPMs based on eligible barrier functions which are neither logarithmic nor self-regular. They obtained so far the best known complexity result based on a specific eligible barrier function for linear optimization(LO). Motivated by their works we define a new class of barrier functions and propose new large-update primal-dual IPMs based on these functions for $P_*(\kappa)$ nonlinear complementarity problems(NCPs). We show that the new IPMs have $O(n^{\frac{24}{43}} \log \frac{n\mu^o}{\epsilon})$ iteration bound for large-update and $O(\sqrt{n}\log \frac{n\mu^o}{\epsilon})$ for small-update methods. For large-update methods the complexity result improves currently the best known bound and for small-update method this is currently the best known bound.

Regularity conditions in second-order cone programs without strict complementarity

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This talk is based on a joint work with C. Kanzow and I. Ferenczi of the University of Würzburg.

Abstract. The optimality conditions of a second-order cone program (SOCP) can be reformulated as a system of nonsmooth equations involving projection mappings onto second-order cones. For both linear and nonlinear SOCPs, we give sufficient conditions for the nonsingularity of the generalized Jacobian of this system, under which a nonsmooth Newton method is locally quadratically convergent. An interesting and important feature of these conditions is that they do not require strict complementarity of the solution.

A modified conjugate gradient algorithm for unconstrained optimization

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Abstract. Conjugate gradient (CG) methods have played special roles in solving large scale nonlinear optimization problems with smooth objective functions $f : R^n \to R$. Search directions in the CG methods are generated by the sequence $d_1 = -\nabla f(x_1)$ and $d_k = -\nabla f(x_k) + \beta_k d_{k-1}$, for $k \geq 2$. By introducing different conjugacy conditions, researchers proposed different formulas for β_k. The related conjugate gradient algorithms may have quite different behaviors for general functions. Recently, Dai and Liao [1] proposed some new nonlinear conjugate gradient algorihms based on the standard secant equation. One of these algorithms is not only globally convergent for general functions but also performs better than some well known conjugate gradient methods. Also, Li et al. [2] introduced some new conjugate gradient methods using the secant equation proposed by Wei et al. [3] with better numerical performance in some cases. Here, we use the modified secant secant equation proposed by Zhang and Xu [4] and using suggestions recently proposed in conjugate gradient algorithms, we introduce a new conjugacy condition and proposed a modified conjugate gradient algorithm. It can be shown that under some proper conditions out modified conjugate gradient algorithm is globally convergent for general functions. Numerical results showed that our algorithm is competitive and sometimes preferable to the recently proposed conjugate gradient algorithms.

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An affine-scaling interior-point CBB method for continuous knapsack constraints

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Abstract. An affine-scaling algorithm for optimization problems with a single linear equality constraint and box restrictions is developed. The algorithm has the property that each iterate lies in the relative interior of the feasible set. The search direction is obtained by approximating the Hessian of the objective function in Newton's method by a multiple of the identity matrix. The approximation given by the cyclic Barzilai-Borwein (CBB) formula yields the ASL-CBB scheme (affine scaling interior point method for linear constraints). Global convergence is established for a nonmonotone line search. The algorithm is particularly well suited for optimization problems where the Hessian of the objective function is a large, dense, and possibly ill-conditioned matrix. As an application, the Support Vector Machine is considered.

A fast interval algorithm based on a binary tree data structure for global optimization

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Abstract. We investigate interval methods as a means for solving global optimization problems and seek to develop a faster, more efficient interval algorithm that can identify multiple global solutions. Our approach is based on a memoryless interval algorithm that was recently reported by the second author. The reported results have indicated that the memoryless interval algorithm significantly improved memory requirement and convergence speed of conventional interval algorithms, while retaining a reasonable degree of reliability. Our present work attempts to improve the reliability of the memoryless interval algorithm while sacrificing little both in memory space usage and in overall speed of convergence. As our main strategy, a binary tree data structure is introduced as a means of memory that would guide the algorithm to locate a new approximate solution, while the overall algorithm employs the memoryless interval algorithm iteratively. Each application of the memoryless interval algorithm is directed by the tree so that no cycling occurs. The combination of the memoryless interval algorithm and the tree data structure offers an effective method to iteratively improve the current best solution. Such a strategy also offers an opportunity to identify multiple global solutions as well. In implementing the new algorithm, we used bisection as a means of branching in the base memoryless interval algorithm. Since the base algorithm is so fast, we knew that we could run the algorithm hundreds or thousands of times and it would still be faster than most traditional interval algorithms. Our challenge was to determine where to begin the next run of the base algorithm so that we could begin the search again. We decided to utilize the binary tree structure to organize our search method in finding global solutions. Each node of the tree holds a Y (the interval vector) and a y (the corresponding lower bound of the returned interval of the inclusion function). The first run of the algorithm fills in a skeleton of the tree, with the original interval vector being the root, and its left child being the interval vector with the associated lower interval and the right child, the upper interval. Whichever one is chosen to be further bisected gets investigated, while the other node is marked as "unchecked" and does not get any left or right nodes. Once the first run of the algorithm is complete, the program looks over all of the "unchecked" childless nodes to find the one with the smallest "y value," and that interval vector is flagged so that we can begin our next run of the algorithm at this location with this interval vector. Thus, with each run, the tree is becoming fuller and more complete. The algorithm is run for a prescribed number of times, which is input by the user. Thus far, we have received positive results from this new algorithm. It has been found to successfully identify global solutions in situations where the base algorithm alone fails. If multiple global solutions exist, it can recognize those other solutions. While not as fast as the base algorithm, this refined algorithm is still relatively quick as compared to many traditional interval methods. Through this paper, we seek to explain our algorithm in greater detail and study its efficiency with the results that we have found through testing various objective functions.

An almost smooth equation reformulation to the nonlinear complementarity problem and related Newton's Method

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Abstract. We convert the nonlinear complementarity problem to a nonsmooth equation. This nonsmooth equation enjoys some nice properties. In particular, it is smooth everywhere except at the solution set. We call this equation an almost smooth equation reformulation to the nonlinear complementarity problem. We present a Newton's method for solving this almost smooth equation. Under appropriate conditions, we prove the global and superlinear/quadratic convergence of the method.

Convex relaxation for nonconvex quadratic programming problems: best D.C. decomposition and SDP formulation

Xiaojin Zheng, Xiaoling Sun and Duan Li
Chinese University of Hong Kong

Abstract. We investigate a general convex relaxation scheme via D.C. decompositions for linearly constrained nonconvex quadratic programming and reveal an equivalence between the "best" parametric D.C. decomposition and its corresponding semidefinite relaxation formulation. We gain dual benefits from this interesting equivalence: (i) Reduction of the iterative dual search process in finding the best D.C. decomposition to a single SDP formulation, and (ii) Identification of a feasible solution of the primal problem by solving the convex relaxation corresponding to the SDP solution.

The maximal correlation problem

Li-Zhi Liao
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Abstract. The maximal correlation problem (MCP) aiming at optimizing correlation between sets of variables plays a very important role in many areas of statistical applications. Currently, algorithms for the general MCP stop at solutions of the multivariate eigenvalue problem (MEP) for a related matrix A. The MEP is a necessary condition for the global solutions of the MCP. Up to date, there is no algorithm that can guarantee convergence to a global maximizer of the MCP, which would have significant impact in applications. In this talk, first, we will report some theoretical results for the global optimality of the MCP. Second, we will present some algorithms which can converge to the global maximal solution of the MCP. Finally, some numerical results will be presented.

Stochastic variational inequality problems with additional constraints and their applications in supply chain network equilibria

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Abstract. This paper considers a stochastic variational inequality problem with additional constraints. Because of existence of the random elements, the problem has no solution in general. First of all, we use the so-called regularized gap function, which is well-known in variational inequality theory, to present a deterministic constrained optimization formulation (called ERM formulation) for the considered problem. Since the ERM formulation contains an expectation, we then propose a quasi-Monte Carlo method and investigate its convergence properties. Furthermore, as an application, we study a supply chain network with restricted output and random demands. We formulate the equilibrium conditions of the supply chain network into a stochastic variational inequality problem with additional constraints. Preliminary numerical experiments indicate that the proposed approach is applicable.

The use of QP-free method in the analysis of slope stability

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Abstract. In the upper bound limit analysis of slope stability based on rigid finite element method, the search for the minimum factor of safety can be formulated as a nonlinear constrained optimization. In generally, the programming problem is a large-scale problem, the unknowns are subject to a highly sparse set of equality constraints based on yield criterion, a flow rule, boundary conditions and energy-work balance equation. It is very difficult to establish an effective solution procedure to find a globally optimum value, and the solution procedure is quite time consuming. Fortunately, the infeasible QP-free algorithm based on exact penalty function and on active-set strategy can be globally convergent toward the KKT points, and the rate of convergence is superlinear or even quadratic. So the optimization problem deduced from upper bound limit analysis of slope stability can be solved by QP-free method, and the global minimum of safety factor can be found more easily. In this paper, we applied firstly QP-free method to obtain solutions for such nonlinear optimization problems, and prompted the upper bound limit analysis approach to become much more practical and powerful for analyzing the slope stability.

An efficient nonstandard simplex algorithm for linear programming

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Abstract. The simplex algorithm travels, on the underlying polyhedron, from vertex to vertex until reaching an optimal vertex. With the same simplex framework, the proposed algorithm generates a series of feasible points (which are not necessarily vertices). In particular, it is exactly an interior point algorithm if the initial point used is interior. Extensive computational experiments show that the algorithm are very ecient, relative to the conventional simplex algorithm, terminating at an 2-optimal vertex, or, if a simple purication is incorporated, at an optimal vertex.

Asymptotic behavior of underlying NT paths in interior point methods for monotone semidefinite linear complementarity problems

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Abstract. An interior point method (IPM) defines a search direction at each interior point of the feasible region. These search directions form a direction field which in turn gives rise to a system of ordinary differential equations (ODEs). Thus, it is natural to define the underlying paths of the IPM as solutions of the system of ODEs. These off-central paths have been shown to be well-defined analytic curves and any of their accumulation points is a solution to the given monotone semidefinite linear complementarity problem (SDLCP). The asymptotic behavior of off-central paths corresponding to a well-known search direction, HKM direction, was also studied. In this talk, we discuss off-central paths corresponding to another well-known direction, the NT search direction. We give necessary and sufficient conditions for when these off-central paths are analytic w.r.t. $\sqrt{\mu}$ and μ, at solutions of a general SDLCP. Also, we present off-central path examples using a simple SDP, whose first derivatives are likely to be unbounded as they approach the solution of the SDP. We work under the assumption that the given SDLCP satisfies strict complementarity condition.

A smoothing approach to the optimisation of traffic networks

Agachai Sumalee, Richard Connors, and David Watling
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Abstract. Transport planners routinely use mathematical models to predict the impacts of network improvements and policy interventions. Methodologies adopted in practice are those available in established software; for urban network analysis this continues to be User Equilibrium (UE). Unfortunately, network optimisation with UE flows is a systematically non-differentiable problem, preventing application of gradient based methods. We can consider a sequence of smoothed versions of the UE network optimisation problem, where successive iterations converge to the original non-smooth problem. This smoothing can be considered as a model of traveller behaviour in its own right, and connects with merit-function smoothing techniques for nonlinear complementarity problems.

A proximal point method for matrix least squares problem with nuclear norm regularization

Defeng Sun
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Abstract. We consider a Newton-CG proximal point method for solving matrix least squares problem with nuclear norm regularization. For the symmetric problem in which the matrix variable is symmetric, the proximal point method is identical to the augmented Lagrangian method applied to the dual problem. For the inner problems in the non-symmetric case, we show that the soft thresholding operator is strongly semi-smooth everywhere, which is a key property for successfully applying a semi-smooth Newton-CG method to solve the inner problems. Numerical experiments on a variety of large scale SDP problems arising from regularized kernel estimation and matrix completion show that the proposed method is very efficient.

[This is a joint work with Kaifeng Jiang and Kim Chuan Toh at National University of University.]

On filter-successive linearization methods for nonlinear semidefinite programming

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Abstract. Using successive linearization method and filter technique, we present a filter-successive linearization method with a trust region-type globalization for solution of nonlinear semidefinite programming. Such a method is based on the concept of filter for nonlinear programming introduced by Fletcher and Leyffer (2002). We describe the new algorithm and prove its global convergence under weaker assumptions. Some numerical results are reported and show that the new method is potentially efficient.

A distributed SDP-based algorithm for large noisy anchor-free graph realization in molecular conformation

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Abstract. We consider the conformation problem of determining the structure of a protein molecule given sparse short-range and noisy distances between atoms. We propose a divide-and-conquer SDP-based algorithm to determine the positions of the atoms (up to translation and rotation). The atoms are recursively partitioned into overlapping groups. When a group is small enough, atom positions are estimated via SDP and refined via gradient descent. Finally we stitch groups together to form a global solution. The algorithm is tested on PDB molecules, and able to compute a structure for a molecule with 13000 atoms, given 30% of the distances less than 6Å(and with 20% noise added) in about 1.5 hour with an RMSD (root-mean-square deviation) of about 1Å.

A smoothing SQP method for nonlinear programs with stability constraints arising from power systems

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Abstract. This paper investigates a new class of optimization problems arising from power systems, called nonlinear programs with stability constraints (NPSC), which is an extension of common nonlinear programs where stability constraints are involved. Since the stability constraint is described generally by eigenvalues or norm of Jacobian matrices of systems, this results that the NPSC to be semismooth. The optimal conditions of both NPSC and its smoothing problem are studied. A smoothing SQP algorithm is proposed for solving the NPSC problems. The global convergence of the algorithm is established. A numerical example from optimal power flow (OPF) is done. The calculating results show the efficiency of the proposed model and the algorithm.

A new exchange method for convex and nonlinear semi-infinite programming

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Abstract. In this talk we propose a new exchange method for solving convex semi-infinite programming (CSIP) problems. We introduce a new dropping-rule in the proposed exchange algorithm, which only keeps those active constraints with positive Lagrange multipliers. Moreover, we exploit the idea of looking for η-infeasible indices of the lower level problem as the adding-rule in our algorithm. Hence the algorithm does not require to solve a maximization problem over the index set at each iteration; it only needs to find some points such that a certain computationally-easy criterion is satisfied. Under some reasonable conditions, the new adding-dropping rule guarantees that our algorithm provides an approximate optimal solution for CSIP problem in a finite number of iterations. As a special case, the quadratically constrained CSIP is also considered. We also purpose this exchange algorithm to non-convex, nonlinear semi-infinite programming problems. Under some different conditions, the algorithm provides an approximate optimal solution for nonlinear semi-infinite programming problems in a finite number of iterations too. In the numerical experiments, we solve some test problems including some numerical examples and some medium size problems from complex approximation theory and FIR filter design to see the effectiveness of the proposed algorithm. We compare our algorithm with existing central cutting plane CSIP algorithm and the SIP solver fseminf in MatLab toolbox, and observe that our algorithm solves CSIP much faster.

On small size linearizations for the quadratic assignment problem

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Abstract. The quadratic assignment problem (QAP) is one of the great challenges in combinatorial optimization. Linearization for QAP is to transform the quadratic objective function into a linear one by introducing additional variables and linear constraints. Numerous QAP linearizations have been proposed, most of which are mixed integer linear programs (MILP). Kaufman and Broeckx's linearization (KBL) is the current smallest one in terms of the number of variables and constraints. Recently, we have presented an efficient linearization which has the same size as KBL. It remains open whether they are the smallest linearizations for QAP. In this article, based on a reductive decomposition presentation of the permutation matrix, we succeed in constructing a smaller linearization for QAP. Numerical comparison is also provided.

Feasibility and solvability of Lyapunov-type linear programming over symmetric cones

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Abstract. In this talk, we are concerned with Lyapunov-type linear programming (LLP for short) over symmetric cones. By introducing and characterizing the generalized inverse of Lyapunov operator over symmetric cones, we establish two kinds of Lyapunov-type Farkas' lemmas to exhibit feasibilities of the corresponding primal and dual problems respectively. As one of the main results, we show that the feasibilities of the primal and dual problems lead to the solvability of the primal problem and zero duality gap under some mild condition. In this case, we obtain that any solution to the pair of primal and dual problems is equivalent to the solution of the corresponding KKT system.

A new Lagrangian net algorithm for solving max-bisection problems

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Abstract. The Max-Bisection problems is an NP-hard combinatorial optimization problem. In this paper, we proposed a new Lagrangian net algorithm for solving the Max-Bisection problems. First, we relax the bisection constraints to the objective function by introducing the penalty function method. Second, a bisection solution is found by a discrete Hopfild neural network (DHNN). The increasing factor can help the DHNN escape from the local minimum. The convergence of the proposed algorithm is also proved. Numerical results of large scale G-set problems show that the proposed method can find a more near optimal solutions.

From the split feasibility problem to the generalized KM theorems

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Abstract. In this talk, I will begin with the Split Feasibility Problem (SFP) and end with the generalized KM theorems. First I show that the SFP can be equivalently formulated as different fixed point problems. Based on these reformulations, several projection-type algorithms are presented or given again but based on new and simpler derivation. Taking the particular form of fixed point operators into account, we give an inexact scheme of an algorithm for the SFP , and a relaxed version of an iterate scheme so that the proposed solution methods can be implemented efficiently. It has been known that the KM iterate is an important algorithm for the general fixed point problem. Inspired by the previous concrete algorithms, we extend the KM iterate so that the some algorithms in the broader fields may be treated or improved in the united framework. Finally we illustrate some applications of the generalized KM theorems.

Nonlinear augmented Lagrangian for nonconvex multiobjective optimization

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Abstract. In this paper, based on the ordering relations induced by a pointed, closed and convex cone with a nonempty interior, we propose a nonlinear augmented Lagrangian dual scheme for a nonconvex multiobjective optimization problem by applying a class of vector-valued nonlinear augmented Lagrangian penalty functions. We establish the weak and strong duality results, necessary and sufficient conditions for uniformly exact penalization and exact penalization in the framework of nonlinear augmented Lagrangian. Our results include several ones in the literature as special cases.

This is a joint work with Chen Chunrong, Cheng T.C.E. and Li S.J. and was partially supported by the Research Committee of The Hong Kong Polytechnic University.

An active set strategy based on augmented Lagrangian method for non-negativity constrained image deblurring problem

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Abstract. In this paper we investigate total variation-based non-negativity constrained image deblurring problems. An active set strategy based on augmented Lagrangian method is presented and its convergence in finitely many steps is proved. Furthermore, we deduce that the active set strategy can be reformulated as a semismooth Newton method for a nonsmooth system of equations.

New necessary optimality conditions for bilevel programming problems

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Abstract. Bilevel programming problem (BLPP) is a sequence of two optimization problems where the constraint region of the upper level problem is determined implicitly by the solution set to the lower level problem. The classical approach to solve such a problem is to replace the lower level problem by its Karush-Kuhn-Tucker (KKT) condition and solve the resulting mathematical programming problem with equilibrium constraints (MPEC). In general the classical approach is not valid for nonconvex bilevel programming problems. The value function approach uses the value function of the lower level problem to define an equivalent single level problem. But the resulting problem requires a strong assumption such as the partial calmness condition for the KKT condition to hold. In this paper we combine the classical and the value function approaches to derive new necessary optimality conditions under rather weak conditions. The required conditions are even weaker in the case where the classical approach or the value function approach alone are applicable. This is a joint work with Daoli Zhu, Fudan Unversity, China.

Gradient method with short BB step-lengths for minimizing large scale convex quadratic functions

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Abstract. The gradient method is one of the most simple methods for solving unconstrained optimization, it has the advantages of easy to program and suitable for large scale problems. Different step-lengths give different gradient algorithm. In 1988, Barzilai and Borwein gave two interesting choices for the step-length and established superlinearly convergence results for two dimensional convex quadratic problems. Barzilai and Borwein's work triggered many researches on the gradient method in the past two decades. In this paper we investigate how the BB method can be further improved. We generalize the convergence result for the gradient method with retards. Our generalization allows more choices for the step-lengths. An intuitive analysis is given on the impact of the step-length for the speed of convergence of the gradient method. We proposed a short BB step-length method. Numerical results on random generated problems are given to show that our short step technique can improve the BB method for large scale and ill-conditioned problems, particularly when high accurate solutions are needed.

Stochastic nonlinear complementarity problems: theory, algorithms and applications

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Abstract. Stochastic nonlinear complementarity problems (SNCPs) root from the classic nonlinear complementarity problems (NCPs) which affected by stochastic factors. Deterministic formulations are needed to deal with the stochastic factors. In this talk, we present some recent results on various deterministic formulations of SNCPs, including the theoretical analysis of existence and boundedness of solution, robustness of solution, efficient algorithms, as well as real applications in traffic equilibrium under uncertainty

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New results on robust stochastic optimization

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(Based on joint work with Li CHEN and Simai HE)

Abstract. The maximal correlation problem (MCP) aiming at optimizing correlation between sets of variables plays a very important role in many areas of statistical applications. Currently, algorithms for the general MCP stop at solutions of the multivariate eigenvalue problem (MEP) for a related matrix A. The MEP is a necessary condition for the global solutions of the MCP. Up to date, there is no algorithm that can guarantee convergence to a global maximizer of the MCP, which would have significant impact in applications. In this talk, first, we will report some theoretical results for the global optimality of the MCP. Second, we will present some algorithms which can converge to the global maximal solution of the MCP. Finally, some numerical results will be presented.

Stream 6

Matrix Computations and Nonlinear Equations

Organizer: Xiaojun Chen
The Hong Kong Polytechnic University, Hong Kong

Plenary Talk

Missing data recovery by tight-frame algorithms

Raymond H. Chan
Department of Mathematics
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Abstract. The recovery of missing data from incomplete data is an essential part of any image processing procedures whether the final image is utilized for visual interpretation or for automatic analysis. In this talk, we first introduce our tightframe-based iterative algorithm for missing data recovery. By borrowing ideas from anisotropic regularization and diffusion, we can further improve the algorithm to handle edges better. The algorithm falls within the framework of forward-backward splitting methods in convex analysis and its convergence can hence be established. We illustrate its effectiveness in few main applications in image processing: inpainting, impulse noise removal, super-resolution image reconstruction, and video enhancement.

Error bounds for complementarity problems

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(joint work with Z. Wang, Nanjing)

Abstract. The complementarity problem consists in finding a vector $x^* \in R^n$ such that

$$x^* \geq 0, F(x^*) \geq 0, (x^*)^T F(x^*) = 0, \quad (1)$$

where $F : R^n \to R^n$. The partial order is defined componentwise. Most algorithms are only computing approximations $\hat{x}$ to x^*. Therefore, it is an important question to bound the error $e(\hat{x}) = \hat{x} - x^*$. The discussion of this problem has started only two decades ago and there exist not so much results. In our talk we will consider the problem (1) with $F(x) = Mx + \varphi(x)$, where M is a (n, n) matrix and φ is a so-called tridiagonal (nonlinear) mapping. This means that the i-th component $\varphi_i(x)$ is only dependent on x_{i-1}, x_i and x_{i+1}, where $x = (x_i) \in R^n$. This problem occurs if we disretize certain free boundary problems. For the case that $\varphi_i(x)$ is only dependent on x_i, $\varphi_i(x) = \varphi_i(x_i)$, we consider the concept of a feasible vector in order to bound a solution. Again the problem occurs with disretized free boundary problems.

Enclosure methods for the matrix square root

Andreas Frommer
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Abstract. The square root function can be extended to $n \times n$ matrices A in the operator theoretic sense if 0 is not a derogatory eigenvalue of A. Computationally, such a square root can be approximated iteratively by using appropriate and stable variants of Newton's method or by using the spectral decomposition, provided A is diagonizable.

In this presentation we consider the task of, given a computed approximate square root M of A, determining a narrow enclosing interval matrix $[M]$ for which we know with mathematical certainty that it contains the exact square root of A. To this purpose we use the Krawczyk operator based on interval arithmetic. If applied naively, the computational complexity will arise to $\mathcal{O}(n^6)$ which grows prohibitively fast. We therefore present and analyze a variant of Krawczyk's method which is based on an appropriate factorization of the Jacobian. This variant achieves a complexity of $\mathcal{O}(n^3)$ when applied to the matrix square root in the case that A is diagonizable. Results will be presented using the Matlab toolbiox INTLAB.

Computation of matrix exponential in the long-time wave field simulation problem for one-dimensional non-periodical sonic crystals

Youhua Fan, Xiaojian Liu
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Abstract. Recentlythere has been a great interest in studying the properties of sonic (phononic) crystals. We find the wave field simulation for one-dimensional non-periodical sonic crystals can be seen as solving a matrix exponential e^{At} when the controlling differential equation is written as the Hamilton's form. For long-time simulation, the computation result of this matrix exponential will have big error because the matrix At (A is non-normal) becomes very large and the general scaling and squaring method dosen't work in this case. By analyzing the eigenvalue and eigenvector properties of the matrix A, we present an algorithm to compute the matrix exponential by engenvalue scaling and matrix diagonalizing. The simulation results shows perfect accuracy of this algorithm.

Rank-deficient nonlinear equations and least squares problems

C. T. Kelley
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Abstract. We discuss two related problems with rank-deficiency for nonlinear problems. We give lower bounds for the conditioning of the Jacobian for pseudo-arclength continuation in the presence of simple fold singularities. We illustrate the results with an application to nuclear engineering. The second part is also an estimate for conditioning. We show how errors in the residual and Jacobian can cause the Levenberg parameter to diverge to infinity in the context of a ill-conditioned nonlinear least squares computation and how the method of subset selection can resolve some of these problems.

A geometric view of Krylov subspace methods on singular systems

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Abstract. We present a geometrical view of Krylov subspace methods applied to singular systems of linear equations $Ax = b$.

First, we will look at the Conjugate Gradient (CG) method for systems where A is symmetric and positive semi-definite. Kammerer and Nashed [1] analyzed the method using operator theory in a Hilbert space setting. We will give a more elementary analysis. Namely, we will decompose CG into the $ran(A)$ and $nul(A)$ components based on the eigenvectors corresponding to the positive and zero eigenvalues, respectively. This shows that the method is essentially equivalent to CG applied to a positive diagonal system in $ran(A)$.

Next, we will analyze the Generalized Minimual Residual (GMRES) method for systems where A is nonsymmetric and singular. We will decompose the algorithm in to the $ran(A)$ and $ran(A)^{\perp}$ components [2] and provide an interpretation of the converegence conditions given in [3], at the same time giving different proofs for the conditions.

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Kantorovich's theorems for Newton's method on Lie groups

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Joint work with J H Wang

Abstract. Let f be a map from a Lie group to its Lie algebra. Under the classical assumptions on f, a convergence criterion of Newton's method (independent of affine connections) to find zeros of a map f is established, and estimates of convergence domains of Newton's method are obtained, which improves the corresponding known results. Applications to optimization problems on Lie group are provided and some known results are extended and improved accordingly.

On the combined perturbation bound for matrix decompositions

Wen Li
South China Normal University
joint work with Weiwei Sun

Abstract. In this talk we present some combined perturbation bound for the polar decomposition, the spectral decomposition and the singular value decomposition, which are almost optimal for each factor.

F-implicit generalized vector complementarity problems

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Abstract. In this talk, we discuss some complementarity problems for F-implicit generalized vector cases. Some existence theorems for the F-implicit generalized vector complementarity problems are obtained. We also present the equivalent relation between F-implicit generalized vector variational inequalities and the F-implicit generalized vector complementarity problems.

Optimizing condition numbers

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Abstract. In this talk, we consider the problem of minimizing condition numbers over a compact convex subset of the cone of symmetric positive semi-definite $n \times n$ matrices. We show that the condition number is a Clarke regular pseudoconvex function. We prove that a global solution of the problem can be approximated by an exact or an inexact solution of a nonsmooth convex program. This asymptotic analysis provides a valuable tool for designing an implementable algorithm for solving the problem of minimizing condition numbers.

A survey on symmetric linear systems of equations with inexact input data

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Abstract. We consider the *symmetric solution* set S_{sym} which is defined as set of all solutions of linear systems $Ax = b$ with a symmetric matrix A, where A and b are allowed to vary within given bounds. This set is obviously a subset of the more familiar *general solution set* S which is defined analogously, but without the restriction of symmetry for A. We give a survey of equivalent descriptions, of properties and of enclosures of S_{sym}. To this end we start with analogues of Hart-fiel's system of inequalities, Beeck's criterion using intersections of sets combined with interval arithmetic, and the famous Oettli Prager cri- terion, which all describe the general solution set S in an equivalent way. It turns out that S_{sym} cannot be described as easily as S. Therefore, one looks for methods to enclose this set by interval vectors, which are not necessarily enclosures for S at the same time. Among others an interval variant of the Cholesky method, a modification of Krawczyk's method due to Jansson, and Rohn's access by means of parameter dependent linear systems provide such enclosures of S_{sym}. They are presented in detail, their properties are discussed, and they are illustrated by examples. Thus, it can be shown that the interval Cholesky method may not be applicable although each symmetric matrix A (within the above mentioned bounds) is positive definite, and hence the traditional Cholesky method is feasible for it. Certain well known equivalences between this algorithm and the Gaussian algorithm do no longer hold. Some open questions in connection with all the presented algorithms are listed.

Convexity of the Krein space numerical range

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Abstract. In 1975, Westwick generalized Hausdorff's conveity theorem on the numerical range of a matrix (1916). His theorem states that the range

$$\{\sum_{j=1}^{n} c_j \langle T\xi_j, \xi_j\rangle : \{\xi_1, \xi_2, \ldots, \xi_n\} \text{is an orthonormal basis}\}$$

is convex for any $n \times n$ matrix T and any real sequence $(c_1, \ldots, c_n)$. We provide an analogous theorem for a Krein space operator and some real sequence.

Moment discretization of ill-posed nonlinear operator equations with weakly bounded noise

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Abstract. We consider nonlinear ill-posed operator equations with noisy data in Hilbert space. However, rather than assuming that the noise is small in the Hilbert space norm, we assume that error is small in the weak sense introduced recently in a paper by P.P. Eggermont, V. N. LaRiccea, and the author, and study what happens when the noise converges weakly to 0.The assumption is made quantitative by sending the noise through a certain compact operator and requiring a strong bound on the image. The nonlinear ill-posed problem is formulated as a moment discretization problem and also as a minimization problem in Hilbert space with Tikhonov penalization. We discuss convergence rates of the regularized minimizers when the operator equation and the nonlinear minimization problem admit effective linearization and quadratic approximations. Some properties of the nonlinear equations that arise from discretization and semi-discretization are explored in the presence of weakly bounded noise.

Variational fuzzy Mumford-Shah model for image segmentation

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Abstract. In this paper, we propose variational fuzzy Mumford-Shah model for image segmentation. In the model, we consider a piecewise smooth image can be decomposed into a smooth function multiplying a piecewise constant function. We employ fuzzy membership functions which allow a pixel to belong to each class with some probabilities in the segmentation framework. In the new segmentation work, we can obtain the image segmentation and other useful information simultaneously such as bias field in medical images or illumination in natural images. We show the existence of minimizers for the proposed energy minimization problem. An iterative algorithm can be developed to solve such energy minimization problem very efficiently. Our experimental results show that the quality of image segmentation results by fuzzy Mumford-Shah model is competitive with those by the other tested segmentation models.

Error free transformations of floating point numbers and its applications

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Abstract. In [1], we have proposed a concept of the error free transformation and developed it in [2]-[3]. In this talk, we will present some applications of the error free transformations such as

P1 Computational Geomertric Algorithms Giving Always Correct Answers,

P2 Applications to Simultanuous Linear Equations,

P3 Inclusion Theorem for Optimum Point of LP,

P4 and Counter Example to Famous Theorem in Nonlniear Circuit Analysis.

This research is supported by the Grant-in-Aid for Specially Promoted Research from the MEXT, Japan: "Establishment of Verified Numerical Computation", (No. 17002012).

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A priori error estimation for accurate matrix multiplication by using optimized BLAS

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Abstract. This talk is concerned with accurate matrix computations, especially, we focus our mind on matrix multiplication by floating-point arithmetic. Recently, we investigated a method which outputs an accurate result of matrix multiplication written in [*Accurate Matrix Multiplication by using Level 3 BLAS Operation*, Proceeding of 2007 International Symposium on Nonlinear Theory and its Applications (NOLTA2008), pp. 508-511]. It is the key technique that two input matrices are split into sum of floating-point matrices without roundoff error, respectively. As for an advantage of the proposed method, level 3 fraction, the amount of matrix multiplication in the proposed method, is very high. Namely, we can efficiently exploit the optimized BLAS like Goto BLAS, Intel Math Kernel Library and ATLAS whose routines for matrix multiplication achieve nearly peak performance. Moreover, these routines automatically use multi-threads. Therefore, our method is also easily parallelized on the Symmetric Multiprocessing (SMP) environment.

In this talk, we introduce a generalized version of the previous work and present an a priori error analysis for this method. From the analysis, we can explain how the method improve the accuracy of the result of matrix multiplication. The more the two input matrices are represent as sum of many matrices, the more the accuracy of matrix multiplication is improved. We can also understand what is a suitable or not suitable structure of the matrix for our method.

A new eigenvalue inclusion set derived from $\alpha 1$-matrices*

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Abstract. It is known that a nonsingularity result about matrices leads to an eigenvalue inclusion result and conversely. Nonsingularity of strictly diagonally dominant matrices and the Geršgorin theorem are two famous results that clearly represent this fact. This idea has been used recently to derive some new eigenvalue inclusion regions. Using this technique we show how to derive a new eigenvalue inclusion set associated with the class of $\alpha 1$-matrices (a subclass of nonsingular H-matrices). In the proof we use a new characterization of $\alpha 1$-matrices that we have recently introduced. We also give some examples which compare some known inclusion sets.

A practical method for computing the largest M-eigenvalue of a fourth-order partially symmetric tensor

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Abstract. In this talk, we consider a bi-quadratic homogenous polynomial optimization problem over two unit spheres arising in nonlinear elastic material analysis and in entanglement studies in quantum physics. The problem is equivalent to computing the largest M-eigenvalue of a fourth-order tensor. To solve the problem, we propose a practical method whose validity is guaranteed theoretically. To make the sequence generated by the method converge to a good solution of the problem, we also develop an initialization scheme. The given numerical experiments show the effectiveness of the proposed method.

Preconditioning for PDE-constrained optimization

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This joint work with Tyrone Rees and Sue Dollar

Abstract. In many instances one requires the repeated solution of partial differential equation problems in order to optimize a design: a typical example would be in the context of the design of aerodynamic structures where the requirement is to solve PDEs for the external flow around a body whilst trying to select its shape to minimize drag.

We will describe the mathematical structure of such PDE-constrained optimization problems and show how they lead to large scale saddle-point systems. We will present new approaches to preconditioning these systems. Numerical results will be given for the simple distributed control for the Poisson equation and for problems where the PDE constraints are provided by the Stokes and Oseen equations for incompressible viscous flow.

Condition number for linear least squares and total least squares problems

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Abstract. Classical condition numbers are normwise: they measure the size of both input perturbations and output errors using some norms. To take into account the relative of each data component, and, a possible data sparseness, componentwise condition numbers have been increasingly considered.

These are mostly of two kinds: mixed and componentwise. In this talk, we give explicit expressions, computable from the data, for the mixed and componentwise condition numbers for the computation of the Moore-Penrose inverse as well as for the computation of solutions and residues of linear least squares problems, total linear least squares problems. In both cases the data matrices have full column (row) rank.

Improved Wilkinson's iteration refinement strategy with roundoff error analysis

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Abstract. Wilkinson's iteration refinement is frequently used for solving the ill-conditioned system of linear algebraic equations $Ax = b$. However it may not work well in some cases. As Wilkinson's refinement can be viewed as applying the explicit Euler method to a dynamic system which has a unique asymptotically stable equilibrium point $x^* = A^{-1}b$, this motivates us to present in this talk an improvement of Wilkinson's refinement by using the implicit Euler method, instead of the explicit one. The implicit Euler method possesses a better stability than the explicit Euler method, and so a better numerical performance of the derived iteration refinement can be expected. We prove that our improved Wilkinson's refinement is unconditionally convergent to the solution of the linear system. Moreover, the roundo analysis is considered for the improved refinement. We perform the numerical experiments for some ill-conditioned linear systems, to compare the new refinement with the original one, numerical results are also reported.

Preconditioners for saddle point problems arising in blood flow dynamics

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This work was supported by NSFC Grant 10801106.

Abstract. The mathematical model of blood flow dynamics in the cardiovas- cular system leads to a saddle point problem, which is based on finite element discrete Navier-Stokes equations coupled with structural mod- els for the vessel walls. We propose two-by-two block preconditioners for the Krylov subspace method for the solution of the saddle point problem. Theoretical analysis show that they give a good approxima- tion of the coecient matrix, and can improve the spectral property of the original saddle point problem. We also provide serval numerical examples to show the efficiency of the preconditioners.

Generalized Newton-iterative methods for nonlinear equations with locally Lipschitzian functions

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Abstract. In this paper, some generalized Newton-iterative methods are proposed to solve nonlinear equations $H(x) = 0$ in which the function H is locally Lipschitzian continuous. The R-linear convergence is obtained for the proposed methods when H is semismooth. Furthermore, the superlinear convergence can also be obtained under some further assumptions on H as well as the numbers of the inner iterates. As examples of the generalized Newton-iterative methods, generalized Newton additive and multiplicative Schwarz iterative methods to solve a semismooth reformulation of linear complementarity problems with an M-matrix are considered.

Workshop 1

Verified Computation of Solutions for Partial Differential Equations and Related Topics

Organizer: Mitsuhiro T. Nakao
Kyushu University, Japan

Enclosures for eigenvalues of selfadjoint and non selfadjoint ordinary differential equations

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Abstract. The solution of many physical problems can be reduced to knowledge of the eigenvalues of selfadjoint, or non selfadjoint ordinary differential equation. In this talk we shall show that enclosures for these may be obtained using an interval based initial value problem solver together with results from oscillation theory for ODE's, asymptotic analysis and complex function theory.

Dynamics of boundary spikes for Gierer-Meinhardt model in 2D

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Abstract. In 1972, Gierer and Meinhardt proposed model equations describing pattern formations in biology according to the mechanism of diffusion induced instability by Turing. The model equation is as follows:

$$\left\{\begin{array}{rcl} A_t & = & d_1\Delta A - A + \frac{A^{a_1}}{H^{a_2}} + a_5, \\ \tau H_t & = & d_2\Delta H - H + \frac{A^{a_3}}{H^{a_4}}, \end{array}\right. \tag{0.5}$$

where d_1, d_2 are positive constants, $a_j \geq 0$ are non-negative constants satisfying

$$0 < \frac{a_1 - 1}{a_2} < \frac{a_3}{a_4 + 1}.$$

By taking $d_2 \to \infty$, we have a simplified version of (0.5) called shadow system:

$$\left\{\begin{array}{rcl} A_t & = & d_1\Delta A - A + \frac{A^{a_1}}{\Xi^{a_2}}, \\ \tau \Xi_t & = & -\Xi + \frac{1}{|\Omega|\Xi^{a_4}}\int_\Omega A^{a_3} dx \end{array}\right. \tag{0.6}$$

for $x \in \Omega \subset \boldsymbol{R}$.

It has been known that for the Gierer-Meinhard model, stable stationary spike solutions exist on the point with maximal curvature of boundaries. In this talk, we rigorously give the equation describing the motion of spike solutions on boundaries for general types of reaction-diffusion systems if the boundaries are gently curved or the shadow system of the Gierer-Meinhardt model. Specially, we can apply the general results to the Gierer-Meinhard model and show that a single spike solution moves toward a point with maximal curvature of boundaries.

For the shadow system (0.6), we can also show multi-spikes are unstable with positive eigenvalue.

A numerical verification method for solutions of nonlinear parabolic problems

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Abstract. By using the projection and the constructive a priori error estimates, a new method for the numerical norm estimation of the inverse of linear parabolic operators is formulated. As a useful application of the result, we present a new verification method of solutions for nonlinear parabolic problems, which enables us to simplify the verification process. Several numerical examples that confirm the actual effectiveness of the method will be presented.

Numerically verified bifurcated solutions of 3 dimenensional Rayleigh-Benard convection problem

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Abstract. Using Nakao's method, we verify bifurcated solutions of 3 dimensional Rayleigh-Benard convection problem numerically. These solutions form branch lines of the bifurcation diagram which are roll, rectangular, and hexagonal types. The first kind of branch can be studied in a reduced 2 dimensional equations, but others are totally 3 dimensional phenomena which resemble the original patterns shown by Benard. The verification method uses the usual fixed point settings after introducing a Newton type operator with interval arithmetic in real computation.

On the constants of a priori error estimates for the H_0^2-projection in Ritz-Galerkin methods

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Abstract. The actual values of constants appearing in the error estimates of projections into approximate subspaces by using spectral methods or finite element methods play an important role in numerical verification methods for boundary value problems (e.g. [2]). In order to satisfy verification conditions, we need to estimate these constants as small as possible. For the H_0^1-projection, several optimal constants are already known (e.g. [1]). However, such a constant of for the H_0^2-projection is not yet considered up to now. In this research, we introduce the constants in a priori error estimates for the H_0^2-projection by spectral methods and finite element methods. The constants we introduce here are very closed to be optimal. Actually, these constants are less than half of the existing value in [3].

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A constructive a priori error estimation for finite element discretizations in a non-convex domain using mesh refinement

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Abstract. In solving elliptic boundary value problem by finite element method in a bounded domain which has a re-entrant corner, the convergent rate could be improved by using mesh refinement. In our research, we have obtained explicit a priori error estimation for finite element solution of the Poisson equation in a polygonal domain. Our result is important in a theoretical sense as well as practical calculations because the constructive a priori error estimation for linear problem are often used for computer-assisted proof for non-linear problems.

For $f \in L^2(\Omega)$, we consider the weak solution of the following partial differential equation.

$$\begin{cases} -\Delta u &= f \quad \text{in} \quad \Omega, \\ u &= 0 \quad \text{on} \quad \partial\Omega. \end{cases}$$

where Ω is the polygonal domain. If Ω is a convex domain, we can obtain a priori error estimation as follows:

$$\|u - u_h\|_{H_0^1(\Omega)} \leq Ch\|f\|_{L^2(\Omega)},$$

, where u_h is a finite element solution, h denotes maximum mesh size, and C is a constant which is calculated only by condition of mesh. However, if Ω is a non-convex domain, we cannot obtain such $O(h)$ error estimation with uniform mesh because of the singularities at the re-entrant corner. To deal with this difficulty, we use mesh refinement and furthermore, obtained a priori error estimation for finite element solutions.

Eigenvalue enclosures and exclosures for non-self-adjoint problems in hydrodynamics

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(joint work with B. M. Brown, M. Marletta, C. Tretter and M. Wagenhofer)

Abstract. In this talk I will discuss computer-assisted proofs of enclosures and exclosures of eigenvalues of various problems in fluid dynamics and quantum mechanics. A brief outline of the algorithm we developed and applied is as follows. The eigenvalue problem is formulated as a problem of finding zeros of an analytic function that is calculated by means of solutions of initial value problems. Using a code to solve differential equations which is based on interval arithmetic one can calculate this analytic function with guaranteed error bounds. We use the argument principle to obtain a guaranteed enclosures of the number of zeros of the analytic function in a given box. This can be used to either enclose eigenvalues in small boxes or to count the number of eigenvalues in a box of any size. The latter can also be used to get eigenvalue exclosures.

We apply the algorithm to various problems in fluid dynamics, in particular, to the Orr–Sommerfeld equation with Poiseuille and Couette profile. For the Poiseuille flow we enclose an eigenvalue in the unstable half-plane of the complex plane for Reynolds number $R = 5772.221818$, which gives a rigorous proof of the instability of the flow. For other Reynolds numbers and wave numbers we can show stability by excluding eigenvalues in some region in the unstable half-plane and using analytic estimates for the eigenvalues. For the Couette flow we obtain some explicit upper bounds on the imaginary parts of eigenvalues, which all lie in the stable half-plane. Moreover, we consider the spectrum that is connected with the problem of natural oscillations of an incompressible inviscid fluid in the neighbourhood of an elliptical flow. In this case the spectrum is continuous. However, by separation of variables this problem can be turned into a family of eigenvalue problems which can be treated simultaneously by our algorithm. This gives an enclosure of the spectrum. Finally, we obtain enclosures of resonances of Schrödinger operators with fast decaying potentials.

Verified numerical computation of a period of unstable periodic orbits for the Rossler system

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Abstract. We describe a numerical computation with guaranteed accuracy to find a period of unstable periodic orbits for the Rossler system. We use the delayed feedback control to stabilize unstable periodic orbits. It is well known that this control dose not change the solution of the original equation corresponding to the unstable periodic orbit. We will show some numerical verification results of the period-one cycle for the Rossler attractor.

Validated continuation and paths of equilibria for infinite dimensional problems

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Abstract. The computation of a parameter dependent family of equilibria (or periodic orbits) of a partial differential equation can be formulated as computing solutions of an infinite dimensional parameter dependent nonlinear operator of the form

$$F(u, v) = 0, \; v \in R.$$

Predictor-correction continuation techniques provide some of the most efficient numerical methods for solving problems of this type. A complication that arises in the case of infinite dimensional problems is that this procedure must be applied to some finite dimensional approximation which, of course, raises the question of the validity of the output. In this talk I will describe a technique which we call validated continuation that combines the information obtained from the predictor-corrector steps with ideas from rigorous computations and verifies that the numerically produced zero for the finite dimensional system can be used to explicitly define a set which contains a unique zero for the infinite dimensional partial differential equation.

A brief description of the technique is as follows. Using regularity conditions on the solutions we derive a set of priori estimates on truncation errors that arise from the reduction to the finite dimensional problem on which we compute. The predictor-corrector computation begins with an approximate solution u_0 at parameter value v_0. The predictor step produces an approximate equilibrium $\tilde{u}_1$ at nearby parameter value v_1, and the corrector step, based on a Newton-like operator T takes $\tilde{u}_1$ as its input and produces, within the prescribed tolerance, a solution u_1 at v_1. The validation is based on the contraction mapping theorem. In particular, the problem is reduced to verifying a finite number of polynomial inequalities, which provide sufficient conditions to have a contraction which define a set in the infinite dimensional space on which an extension of T is a contraction mapping. Extensions of this method allow one to rigorously determine paths of solutions. I will conclude with recent applications of this method to a variety of problems including the proof of chaotic dynamics in a family of ordinary differential equations.

Numerical stability analysis of periodic solutions of ordinary differential equations

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Abstract. One of standard methods to systematically study complicated bifurcation phenomena in nonlinear systems is to examine stability of steady states, for example, equilibrium points and periodic solutions. This work considers numerical stability analysis of periodic solutions of ordinary differential equations.

We can determine stability of periodic solutions using Floquet multipliers which are eigenvalues of the matrix solution of variational equations. Some numerical methods to simultaneously solve ordinary differential equations and the corresponding variational equations have been developed. But it has been reported that commonly used numerical methods can produce incorrect results under some conditions. This work proposes a new method to control errors of solutions of the variational equations and to reduce round-off errors in computing eigenvalues of the matrix solution, namely Floquet multipliers. Numerical examples show that the proposed method works very well even under some severe conditions for which conventional methods yield erroneous results.

Since the basic idea of the proposed method is to iteratively solve the variational equations, we may expect that accuracy of computed results can be numerically verified using this formulation.

Orbital stability investigations for travelling waves in a nonlinearly supported beam

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Abstract. We consider the fourth-order problem

$$\varphi_{tt} + \varphi_{xxxx} + f(\varphi) = 0, \quad (x,t) \in \mathbb{R} \times \mathbb{R}^+, \tag{0.7}$$

with a nonlinearity f vanishing at 0. Solitary waves $\varphi = u(x + ct)$ satisfy the ODE

$$u'''' + c^2 u'' + f(u) = 0, \tag{0.8}$$

and for the case $f(u) = e^u - 1$, the existence of at least 36 travelling waves was proved in [1] by computer assisted means.

By [2], u is *stable* if and only if the function

$$d(c) := \frac{1}{2}\int_{\mathbb{R}} (u'')^2 - \frac{c^2}{2}\int_{\mathbb{R}} (u')^2 + \int_{\mathbb{R}} F(u), \tag{0.9}$$

where $F'(u) = f(u)$, is strictly convex in a neighborhood of c, and *unstable* if and only if the function $d(\cdot)$ is strictly concave in a neighborhood of c. In this talk we present a method to check these conditions rigorously by computer-assistance.

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Numerical existence theorem for solutions of fixed point type equations and its applications

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Abstract. In [1], we have proposed the numerical existence theorem for fixed point type equations. In this talk, we will present some applications of this theorem such as

P1 Boundary value problems of ODE,

P2 Lippmann-Schwinger equation for sound scattering problem, etc.

This research is supported by the Grant-in-Aid for Specially Promoted Research from the MEXT, Japan: "Establishment of Verified Numerical Computation", (No. 17002012).

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A computer-assisted existence and multiplicity proof for travelling waves in a nonlinearly supported beam

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Abstract. For a nonlinear beam equation with exponential nonlinearity, we prove existence of at least 36 travelling wave solutions for the specific wave speed $c = 1.3$. This complements known results in [2] stating that for almost all $c \in (0, \sqrt{2})$ there exists at least one solution. Our proof makes heavy use of computer assistance: Starting from numerical approximations, we use a fixed point argument to prove existence of solutions "close to" the computed approximations.

One of the open problems which we mentioned in [1] is the question of the stability of those solutions. Such stability investigations, also by computer-assisted means, are presently in progress, as explained in detail in K. Nagatou's lecture.

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A numerical convergence study of an energy stable finite element scheme for two-fluid flow problems

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Abstract. We have developed an energy stable finite element scheme for two-fluid flow problems with surface tension [1]. Each flow is governed by the Navier-Stokes equations. We have performed numerical simulations of rising bubble and falling droplet problems to recognize the robustness and the applicability of the scheme [2]. The scheme is stable in the sense of energy if an integral of the square of approximate curvature on the interface remains bounded. To the best of our knowledge there is no numerical scheme for two-fluid flow problems with surface tension whose solution is proved to be convergent to the exact one. Here we construct manufactured solutions to generalized two-fluid flow problems to examine numerical convergence of the scheme. Our numerical result shows that the energy stable scheme has a nice convergence property. It seems that there has been no manufactured solution for two-fluid flow problems. The manufactured solutions mentioned above will be also useful to check computational codes for two-fluid flow problems.

An iterative scheme for free boundary problems defined with the Hadamard variation

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Abstract. Suppose that we are dealing with functionals defined with a unique solution of an elliptic boundary value problem. If the boundary of the region of BVP is perturbed, then the solution of the BVP and the value of the functionals are also perturbed. Variations with respect to boundary perturbations are called the **Hadamard variation**. If we try to design an iterative scheme for a free boundary problem and analyze its behavior, we need to know the Hadamard variations of the problem. In this talk we consider the **filtration problem** (sometimes, it is called the **dam problem**) and its Hadamard variation. We compute the first and second variations of the functionals related to the variational principle of the filtration problem. We then present an iterative numerical scheme for the problem using the obtained Hadamard variations. Numerical examples and some analysis of the scheme will be given.

This is a joint work with Prof. Takashi SUZUKI, Graduate School of Engineering Science, Osaka University.

Error bound for differential linear variational inequality

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(joint work with X. Chen Department of Applied Mathematics The Hong Kong Polytechnic University)

Abstract. The differential linear variational inequality (DLVI) is a new mathematical paradigm which consists of a system of ordinary differential equations (ODE) and a parametric linear variational inequality as the constraint. The right hand side function in the ODE is not differentiable and the function value can not be computed exactly. Existing numerical methods provide only approximate solutions. In this talk we present an error bound of an approximate solution delivered by the time-stepping method, which includes all discretization and roundoff errors, and so is guaranteed. Numerical examples are given to illustrate the efficiency of the error bound.

An eigenvalue excluding method for the Orr-Sommerfeld problem

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Abstract. Consider the Orr-Sommerfeld equation of the form

$$\begin{cases} (-D^2+a^2)^2u + iaR[V(-D^2+a^2)+V'']u = \lambda(-D^2+a^2)u \text{ on } \Omega, \\ u(x_1)=u(x_2)=u'(x_1)=u'(x_2)=0, \end{cases}$$

where $D = d/dx$ stands for the derivative, $\Omega = [x_1, x_2]$, i is the imaginary unit, $a > 0$ is the wave number of the perturbation, and $R > 0$ is the Reynolds number of an underlying fluid which moves in a stationary flow with given real-valued flow profile $V \in C^2(\Omega)$.

The equation arises when two-dimensional perturbations of the velocity profile are considered, where the stream function ψ is given by $\psi(x, z, t) = u(x)e^{ia(z-ct)}$. Here, $u(x)$ means the amplitude and $c = c_r + ic_i$ is the complex wave speed, and the eigenvalue parameter $\lambda = \lambda_r + i\lambda_i \in \mathbb{C}$ is determined by $\lambda = iaRc$.

The Orr-Sommerfeld equation is a non-selfadjoint eigenvalue problem for the eigenpair (λ, u), and within the frame of linearized stability theory, the flow is stable if the spectrum is located in the right complex half-plane, otherwise unstable.

We have proposed a numerical verification procedure which *encloses* an eigenpair of the Orr-Sommerfeld equation with plane Poiseuille flow. The method uses numerical means, but all numerical errors are taken into account, and hence the method implies a rigorous proof of all statements made. For some fixed Reynolds number and wave number $[a, R]$ we have enclosed an eigenpairs.

This talk will desribe an eigenvalue *excluding* method for the Orr-Sommerfeld problem with Poiseuille flow which should be an important information to clarify eigenvalue structure or the critical curve.

This is joint work with Kaori Nagatou (Kyushu University), Michael Plum (Karlsruhe University) and Mitsuhiro T.Nakao (Kyushu University).

An application of the Lohner method for boundary value problems of ODEs

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Abstract. The Lohner method is most frequently used in validated computation for initial value problems of ODEs. It has a lot of applications, especially on dynamical systems.

For boundary value problems of ODEs, there are not so many applications of validated computaion. One of the authors reported some application of the Nakao method to validated computation of boundary valued problems, in which the accuracy is up to the second order with respect to the time step size because of the use of linear interpolation. Higher order interpolation will give higher accuracy, but it is a future work up to this time.

R.J Lohner applied his method to boundary problems in [1], which can give higher accuracy than the second order of the time step size. Here, by himself, it is pointed out that the way of the application needs interval matrices for systems which should be solved by validated computation, and that this may cause some difficulty in actual computation. The sizes of the systems depend on the number of time steps and are usually large. The cpu time for solving such large size interval systems will become terribly long.

The authors will discuss

- An application of the Lohner method using non-interval matrices in the systems and comparison with the original method
- A device for solving the systems by validated computation within less cpu time
- Semiautomatic formulation for installing programs using INTLAB and MAPLE.

[1] R.J.Lohner, *Enclosing the solutions of ordinary initial and boundary value problems*, In: Kaucher, C.U.E., Kulisch, U.(Eds.), Computer Arithmetic: Scientific Computation and Programming Languages, Teubner, Stuttgart, 1987

Workshop 2

The Interface Problem and Its Applications

Organizer: Yanping Lin
The Hong Kong Polytechnic University, Hong Kong

Recent studies of direct and inverse problems for Maxwell's equations and applications

Gang Bao
Department of Mathematics Michigan State University

Abstract. The speaker will discuss recent developments and challenges on a selected set of research topics, such as three-dimensional electromagnetic wave propagation in periodic chiral or nonlinear structures; inverse diffraction problems; inverse scattering/source problems via uncertainty; numerical techniques for solving linear and nonlinear Maxwell's equations; and multiscale modeling and computation of optical responses of nano structures.

A generalized discontinuous Galerkin (GDG) method for Schrodinger equations with nonsmooth solutions with application in optical waveguides

Wei Cai
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Abstract. In this talk, we present a new generalized discontinuous Galerkin (GDG) method for Schrodinger equations with nonsmooth solutions. The numerical method is based on a reformulation of Schrodinger equations, using split distributional variables and their related integration by parts formulae to account for solution jumps across material interfaces. The proposed GDG method can handle time dependent and nonlinear jump conditions. Numerical results for 1D and 2D time dependent Schrodinger equations validate the high order accuracy and the flexibility of the method for various types of interface conditions. Moreover, modeling of wave propagations in various optical fibers using a full vectorial GDG-BPM (beam propagation) is also presented.

Computational multiscale modeling of electromagnetics

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Abstract. The ongoing rapid progress in the synthesis of a variety of different kinds of nanostructures with fascinating physical properties irreducible to properties of bulk media symbolizes a fundamental breakthrough in the physics and chemistry of condensed matter, significantly extending our knowledge of the nature of solids and our capabilities to control their properties. Solid state nanostructures are constitutive and geometric nanononhomogeneities in semiconductor and dielectric mediums. Fullerenes and nanotubes, semiconductor structures with reduced dimensionality-quantum wells, wires and dots, sculptured thin films, CMOS transistor and photonic crystals can be mentioned as examples.

The main issues of this talk include:

1. The relationship between microscopic Maxwell's equations and macroscopic Maxwell's equations.

2. Scale invariance and mathematical modeling of electromagnetics at nano-scale.

3. Multiscale modeling computation and analysis for the Maxwell's equations in heterogeneous media.

This talk is based on the joint work with Prof.J.Z. Cui, Prof.C.Y. Wang, Prof.W. Allegretto, Prof. Y.P. Lin, Prof.Y.S. Wong and my students: Y. Zhang, L. Zhang and J.Z. Huang.

This work is supported by National Natural Science Foundation of China, Special Funds for Major State Basic Research Projects of China and by NSERC
(Canada).

Ion thruster simulation using immersed finite element particle-in-cell method

Yong Cao
Graduate School at Shenzhan Branch Harbin Institute of Technology

Abstract. A new particle-in-cell algorithm based on three-dimensional immersed finite element method was developed for plasma simulations involving complex boundary conditions. The new simulation model is used in two applications which are of great importance to the development of ion propulsion technology: the ion optics performance and the interaction between spacecraft and the ion thruster. For ion optics simulations, simulations are performed to investigate ion optics plasma flow for a whole subscale NEXT ion optics. The operating conditions modeled cover the entire cross-over to perveance limit range. The results of the ion optics simulations demonstrated good agreement with the available experimental data. For ion thruster plume simulations, simulations are performed to investigate ion thruster plume - spacecraft interactions for the Dawn spacecraft. Plume induced contaminations on the solar array are studied for a variety of ion thruster configurations including multiple thruster firings.

Investigation of uncertainties in nonlinear aeroelastic systems

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Abstract. The study of nonlinear aeroelastic systems is important in dynamic response investigations of aircraft structures. However, in reality uncertainties are presence in one form or the other. The uncertainties may arise due to the limitations of the mathematical model in representing the physical system, and/or the uncertainties in the system parameters. In many instances, simulation solutions using the deterministic model may leads to insufficiently accurate results. The key challenge to develop accurate and reliable simulations is to incorporate the effects due to uncertainties. In general, the traditional stochastic approach such as the Monte Carlo Simulations (MCS) requires a tremendous computational cost due to its slow convergence. Recently, more efficient computational programs such as the Stochastic Galerkin Method (SGM), Polynomial Chaos (PC) and Wiener Chaos Expansion (WCE) have been investigated to study the nonlinear behavior of aeroelastic systems with random parameters. It has been reported that for the limit cycle oscillations and Hopf bifurcations, the use of the discrete wavelet transformation gives accurate predictions for the stochastic aeroelastic behavior.

In this paper, we propose a simple but efficient technique based on the Stochastic Collocation Method (SCM), which can be regarded as a special kind of sampling based method combining the strength of the Monte Carlo Simulation and the Stochastic Galerkin Method. The convergence of the solution with respect to the number of the nodal points is investigated, and it has been shown that the proposed method reduces the computational significantly compared to those based on the MCS. In the investigations of the limit cycle oscillations and Hopf bifurcations in an aeroelastic model, the predictions based on the SCM is at least as accurate as those using the Wavelet Chaos Expansion. However, the SCM is straightforward to implement, and flexible to incorporate the uncertainties. Simulation results using the SCM and other stochastic approaches based on MCS, PC and SGM for nonlinear aeroelastic response will be compared and reported. The proposed SCM is currently being investigated for the secondary bifurcations in which the uncertainties are resulted from the nonlinear coefficient in the structure term and also from the initial condition in the pitch DOF.

A multi-mesh finite element method for interface problem simulations

Yana Di
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Abstract. For interface problems which give rise to coupled systems of partial differential equations, different components of the solution exhibit a strongly different local behavior. An optimal discretization should use a mesh for each component. We propose an efficient multi-mesh adaptive finite element method which approximates different components of the solution on different h-adaptive meshes.

An optimal quadratic spline collocation method for the biharmonic Dirichlet problem

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Abstract. We present a quadratic spline collocation (QSC) method for the solution of the biharmonic Dirichlet problem

$$\Delta^2 u = f \text{ in } \Omega, \quad u = \partial u/\partial n = 0 \text{ on } \partial\Omega,$$

where Δ is the Laplacian, Ω is the unit square $(0,1)\times(0,1)$ with boundary $\partial\Omega$, and $\partial/\partial n$ is the outward normal derivative on $\partial\Omega$. We consider the mixed approach in which the problem is reformulated as a coupled system of two Poisson equations by introducing the variable $v = \Delta u$ to obtain

$$\Delta u = v, \quad \Delta v = f \text{ in } \Omega, \quad u = \partial u/\partial n = 0 \text{ on } \partial\Omega.$$

The method is based on an optimal QSC scheme, defined on a uniform partition, for Poisson's equation in Ω with Dirichlet boundary conditions which can be solved efficiently using fast Fourier transforms. Numerical results demonstrate the optimal accuracy in the global maximum norm of the approximations to u and v and their first derivatives, and superconvergence phenomena. In particular, the approximations to u and v are fourth order accurate at the partition nodes, which is comparable accuracy to that of the cubic spline method of Abushama and Bialecki. The efficiency of the scheme is also examined and comparisons with the other methods presented.

High order finite difference schemes for wave equations in inhomogeneous media

Kazufumi Ito
Department of Mathematics
North Carolina State University, USA

Abstract. A higher order method for wave equations in inhomogeneous media is discussed. The method is based on the MAC grids and the sharp interface treatment for discontinuous media is derived. A local defect correction near the interface is developed using the immersed interface method.

Optimal convergence analysis of an immersed interface finite element method

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Abstract. We analyze an immersed interface finite element method based on linear polynomials on noninterface triangular elements and piecewise linear polynomials on interface triangular elements. The flux jump condition is weakly enforced on the smooth interface. Optimal error estimates are derived in the broken H^1-norm and L^2-norm.

A front-tracking method for motion by mean curvature with surfactant

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Abstract. In this talk, we present a finite difference method to track a network of curves whose motion is determined by mean curvature. To study the effect of inhomogeneous surface tension on the evolution of the network of curves, we include surfactant which can diffuse along the curves. The governing equations consist of one parabolic equation for the curve motion coupled with a convection-diffusion equation for the surfactant concentration along each curve. Our numerical method is based on a direct discretization of the governing equations which conserves the total surfactant mass in the curve network. Numerical experiments are carried out to examine the effects of inhomogeneous surface tension on the motion of the network, including the von Neumann law for cell growth in two space dimensions.

Numerical convergence and physical fidelity analysis for Maxwell's equations in metamaterials

Jichun Li
Univ. of Nevada Las Vegas and UCLA

Abstract. In this talk, we discuss a leap-frog mixed finite element method for solving Maxwell's equations resulting from metamaterials. Our scheme is similar to the popular Yee's FDTD scheme used in electrical engineering community, and is preferable for three dimensional large scale modeling since no storage of the large coefficient matrix is needed. Our scheme is proved to obey the Gauss's law automatically if the initial fields satisfy that. Furthermore, the conditional stability and optimal error estimate for the proposed scheme are proved. To our best knowledge, we are unaware of any other publications devoted to the convergence analysis of this leap-frog explicit scheme for Maxwell's equations even in a simple medium, while our results for metamaterials automatically reduce to the standard Maxwell's equations in air by dropping some terms resulting from the constitutive equations.

Immersed finite element methods for elliptic and elastic systems with interfaces and non-homogeneous jump conditions

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Abstract. New finite element methods based on Cartesian triangulations are presented for one and two dimensional elliptic and elastic interface problems involving discontinuities in the coefficients in the solution. The triangulations in these methods do not need to fit the interfaces. The basis functions in these methods are constructed to satisfy the interface jump conditions either exactly or approximately. Both non-conforming and conforming finite element spaces are considered. Corresponding interpolation functions are proved to be second order accurate in the maximum norm.

For non-homogeneous jump conditions, we have developed a new strategy to transform the original interface problem to a new one with homogeneous jump conditions using the level set function.

Splitting domain decomposition methods for porous media flows over non-overlapping sub-domains and interfaces

Dong Liang
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Abstract. In this talk, we consider the time-dependent problems in compressible fluid flows in porous media, which are very important in science and engineering such as groundwater contamination modeling, environmental protection, and reservoir simulation, etc. Numerical simulation of problems in compressible fluid flows in porous media is very challenging due to the coupling, nonlinearity, convection dominance, large scale field and long term prediction. For solving efficiently these problems, we develop new splitting domain decomposition methods (S-DDM) over sub-domains and interfaces by combining the non-overlapping domain decomposition and the splitting technique. At each time step, the S-DDM scheme is applied to solve the water head and concentration equations, in which we propose efficient local multilevel schemes for computing the values on interfaces and the splitting implicit schemes for computing the interior values in sub-domains. Numerical experiments and theoretical analysis are performed and analyzed to show the efficiency and accuracy of the developed S-DDM technique to time-dependent problems in porous media. Our S-DDM technique takes the excellent attractive advantages of both the non-overlapping domain decomposition method and the splitting technique. It reduces computational complexities, large memory requirements and long computational durations. The developed method is suitable and powerful for parallel computing for realistic long term and large scale simulation of compressible fluid flows in porous media.

IFE methods for solving interface problems on Cartesian meshes with local refinement

Tao Lin
Department of Mathematics
Virginia Polytechnic Institute and State University

Abstract. In this talk, we discuss the applications of immersed finite element (IFE) and discontinuous Galerkin (DG) formulation to the boundary value problems of the popular 2nd order elliptic equation with discontinuous coefficient referred as interface problems. The combination of the immersed finite element and the DG formulation leads to numerical methods with two distinct features: (a) their meshes can be formed independent of the material interface even if the interface has a nontrivial geometry; hence Cartesian meshes can be use if desired; (b) local mesh refinement can be easily implemented with Cartesian meshes, especially at the locations around the material interfaces. We will present a class of specific DGIFE methods that can use the DG formulation strategically only at the locations needed while keeping the total computational cost down to a level comparable to the usual Galerkin finite element method.

On the fast linear solvers for Laplace transformation methods for parabolic problems

Dongwoo Sheen
Seoul National university

Abstract. We will discuss the method of Laplace transformation to solve several parabolic problems. First parabolic problems will be transformed to a set of complex-valued elliptic problems on suitable contours by the Laplace transformation. For these Helmholtz-type complex-valued elliptic problems can be solved in parallel. Then the original time-dependent solutions can be obtained by suitable Laplace inversion. In this talk we will discuss and compare fast linear solvers such as multigrid methods, the QMR (quasi-minimal residual) algorithm, and other numerical methods. Applications will include efficient numerical calculation methods for option pricing.

An Eulerian-Lagrangian formulation for porous medium flow

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Abstract. Many difficult problems arise in the numerical simulation of complex fluid ow processes in reservoir simulation, subsurface contaminant transport and remediation, and other applications. The mathematical models used to describe these fluid ow processes are coupled systems of nonlinear advection-diffusion equations, which are advection-diffusion type with advection being the dominant process, and constraining equations. Due to the nonlinearity and couplings of these equations, the moving steep fronts and complicated structures present in the solutions to these systems, the singularities of the solutions at sources and sinks, the numerical treatment of these systems often encounters severe difficulties. In this talk, we discuss Eulerian-Lagrangian methods for the numerical simulation of multiphase, multicomponent compositional ow and transport. Our numerical experiments show that the resulting numerical scheme generates stable and physically reasonable numerical solutions. Finally, convergence analysis for the Eulerian-Lagrangian methods will be outlined.

On numerical solution of free boundary problems arising from option valuation

Song Wang
School of Mathematics & Statistics The University of Western Australia Perth, Australia

Abstract. In this talk I will present some of our latest advances in the numerical solution of free boundary problems arising from pricing various options tradable in financial markets. These include penalty methods for a complementarity problem and an HJB equation and some discretization methods for solving the penalized problems. Both theoretical and numerical aspects of the methods will be addressed.

Interface and polynomial eigenvalue problems in quantum dots simulations

Weichung Wang
Department of Mathematics National Taiwan University

Abstract. Numerical simulations of nanoscale semiconductor quantum dots in various geometric structures play an essential role for investigating the quantum dots' energy spectrum and wave functions. Simple yet efficient finite-difference and finite-volume schemes are first developed to discretize the three-dimensional Schrodinger's equation and the corresponding interface conditions. Jacobi-Davidson type algorithms for computing interior eigenpairs of the resulting large-scale polynomial eigenvalue problems are then proposed and explored. Computational results demonstrate efficiency and robustness of the proposed schemes and further suggest several physical predictions.

Adaptive anisotropic finite element mesh refinement for interface problems

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Abstract. In this paper, we discuss the numerical methods of the interface problems. The standard conforming finite element methods are used, and a kind of a posteriori error estimators is constructed. These a posteriori error estimators not only provide the information on the distribution of the error but also show some hints on the mesh refinement direction. Based on the new a posteriori error estimators, the adaptive anisotropic finite element mesh refinement can be applied. Numerical examples show that the new schemes are more efficient than the adaptive isotropic finite element methods for the interface problems.

Superconvergence estimates of finite element methods for American options

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Abstract. In this paper we are concerned with finite element approximations to the evaluation of American options. Firstly, following W. Allegretto etc, SIAM J. Numer. Anal. 39 (2001), 834–857, we introduce a novel practical approach to the discussed problem, which involves the exact reformulation of the original problem and the implementation of the numerical solution over a very small region, such that this algorithm is very rapid and highly accurate. Secondly, by means of a superapproximation and interpolation postprocessing analysis technique, here we present the sharp L^2-, L^∞-norm error estimates and the H^1-norm superconvergent estimate, respectively, for this finite element method. As a by-product, the global superconvergence result can be used to generate an efficient a posteriori error estimator. Some numerical examples are presented to demonstrate our theoretical results.

Workshop 3

Data Mining and Business Intelligence

Organizer: Yong Shi
Graduate University of Chinese Academy of Sciences, China and University of Nebraska at Omaha, USA

Integration of classification and pattern mining: a discriminative and frequent pattern-based approach

Hong Cheng
Department of Systems Engineering and Engineering Management
The Chinese University of Hong Kong

Abstract. Classification is a core method widely studied in machine learning, statistics, and data mining. Many classification methods assume that the input data is in a feature vector representation. However, in many tasks, the predefined feature space is not discriminative enough to distinguish different classes. More seriously, in many other applications, the input data, such as those in the form of transactions, sequences, graphs, and semi-structured data, may have no clear, predefined feature vectors. In both scenarios, a primary challenge is how to construct a discriminative and compact feature set. I will talk about the framework of discriminative frequent pattern-based classification and examine the classification accuracy, mining efficiency as well as applications of this method. Open problems and future directions will also be outlined.

Expert mining and its applications

Jifa Gu*, Wuqi Song** Zhengxiang Zhu**, Yijun Liu***
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Abstract. Meta-synthesis system approach (MSA) was proposed by Qian, Yu and Dai in 1990 for solving the open complex giant system problems. MSA wishes to integrate data, information, knowledge, model, experience and wisdom with the help of advanced information technologies. It stands for combination of computer and human emphasized on human. Starting from 1999 NSF of China had supported a major project, which studied the methodological, technological and engineering support of meta-synthesis-based macro-economic decision-support. The one of key research topics in this project is how can we synthesize the opinions from different experts. During investigating the economic system decision problems we had proposed some theories, methods and tools for synthesizing the expert's opinions, such as knowledge transferring from tacit to explicit, consensus building, group argumentation environment (GAE). In 2005 when we were facing to solve some social stability problems, from one side we met with some problems with the large amount of data, information and knowledge, and we found that we should use the data mining, text mining and web mining, from other side we found with the help of computer we may use these data, information and knowledge to construct a lot of models which may give us comprehensive description of social phenomena with the time and space, and for some simulation models even we may create some new data generated from computer according to some rule, model also may forecasts some new results, thus we call it model mining. In social problems people has some behavior, which is tacit, but fit with some psychological knowledge, in this case we shall use the psychology mining. Finally we find that all the data, information, knowledge, results from the models and psychological investigation should be judged, evaluated, analyzed and used by human-experts. Based on the previous research and practice we proposed the expert mining. We develop the theory, methods and tools for expert mining and apply them to solve some problems in the social system and human body system... Especially the later system is close related to the Traditional Chinese Medicine (TCM) doctors, which accumulates not only data, cases, knowledge and information, but also experiences and oriental culture.

A new decomposition algorithm for training bound-constrained support vector machines

Lingfeng Niu and Ya-xiang Yuan
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Abstract. This work proposes a new decomposition algorithm for training bound-constrained Support Vector Machines. A new working set selection rule together with the global convergence base on this rule are given. In order to make the algorithm efficient in practice, projected gradient algorithm and interior point method are combined together to solve the quadratic subproblem. Numerical results on several public data sets validate the correctness and efficiency of the proposed algorithm.

Classification of ambiguous medical data

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and Erhun Kundakcioglu.

Abstract. Support Vector Machines (SVMs) are a set of learning algorithms widely used for classification and regression in data mining, machine vision, and bioinformatics. In this study, SVMs are considered within the multiple instance learning context, where data is composed of bags of instances. This setting is particularly useful when there is ambiguity in the data set (e.g., noise in clinical measurements), thus a selection process among bags of alternatives is necessary. We first extend the SVM formulation to multiple instance data and prove the problem is NP-hard. We propose an exact algorithm and present computational results on image annotation, molecular activity prediction, and breast cancer prognosis data sets. An efficient heuristic is also proposed for multiple instance classification and applied to neural data from a visuomotor categorical discrimination task to classify highly cognitive brain activities.

Pari-mutuel markets: mechanisms and performance

So Man-Cho
Anthony, the Chinese University of Hong Kong

Abstract. Recently, there has been an increase in the usage of centrally managed markets which are run by some form of pari-mutuel mechanism. A pari-mutuel mechanism is characterized by the ability to shield the market organizer from financial risk by paying the winners from the stakes of the losers. The recent introduction of new, modified pari-mutuel methods has spurred the growth of prediction markets as well as new financial derivative markets. Coinciding with this increased usage, there has been much work on the research front which has produced several mechanisms and a slew of interesting results. We will introduce a new pari-mutuel market-maker mechanism with many positive qualities including convexity, truthfulness and strong performance. Time permitting, we will discuss and compare the performance of some of the existing pari-mutuel market-maker mechanisms.

Kernel regularized multiple criteria linear programming

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Abstract. Based on our proposed regularized multiple criteria linear program (RMCLP) for binary classification problems, this paper extends this method to treat with nonlinear case. By applying dual theory, we derived the dual problem of optimization problem constructed in RMCLP, and then proved the solution of RMCLP can be computed by the solution of its dual problem, finally, we constructed Algorithm Kernel RM- CLP by introducing Kernel functions in RMCLP. Furthermore, the paper describes some mathematical properties of this new algorithm. Finally, a series of experimen- tal tests are conducted to illustrate the performance of the proposed Kernel RMCLP with the existing methods: MCLP, multiple criteria quadratic program (MCQP), and support vector machine (SVM). The results of several publicly available datasets and a real-life credit dataset all show that our Kernel RMCLP is a competitive method in classification.

The maximum principles for partially observed stochastic recursive optimal control problem and application

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joint with Dr. Guangchen Wang

Abstract. In this talk, we give a maximum principle for partially observed stochastic recursive optimal control problems under the assumption that control domains are not necessarily convex and forward diffusion coefficients do not contain control variables. Such kind of recursive optimal control problems have wide applications in fiance and economics such as recursive utility optimization and principal-agent problems. By virtue of a classical spike variational approach and a filtering technique, the maximum principle is obtained, and the related adjoint processes are characterized by the solutions of forward-backward stochastic differential equations in finite-dimensional spaces. Then our theoretical results are applied to study a partially observed linear-quadratic recursive optimal control problem. In addition, for the case with initial and terminal state constraints, the corresponding maximum principle is also obtained by using Ekeland's variational principle.

A system for China-based bonded manufacturing enterprises to manage customs risks in global supply chain

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Abstract. Enterprise customs risks refer to uncertainties or unpredictable events encountered by enterprises in complying customs regulations. Currently, over 100,000 enterprises in China are operating bonded manufacturing business. Their production and logistics activities (from procurement of bonded raw materials through component fabrication to delivery of finished products) must be strictly supervised by China Authorities (e.g. China Customs). Any inconsistence or errors in customs registration, declaration, clearance and reconciliation will lead to customs penalties, legal responsibilities, or time delay in fulfilling production/delivery orders, which greatly increase the cost of their logistics and supply chain management. In this paper, a system is developed to help these enterprises to evaluate and manage their customs compliance risks in global supply chain. Designed using service-oriented and event-driven architecture, the system consists of a data integration engine, an active risk data repository, a complex event processing engine, a risk analysis engine and a user friendly interface. Through a series of key customs risk indicators calculated using the data extracted from enterprise information systems, the system not only enables enterprise customs managers to identify the customs risks automatically from daily business operations, but allows them to visualize customs risk levels on demand or in real time. Risk alerting messages also can be sent out to related decision makers for taking proactive measures. One pilot project using the system is implemented at one of our industrial partners. The effectiveness and efficiency of the system is validated by the company's customs department.

Transfer learning in data mining

Qiang Yang
Hong Kong University of Science and Technology

Abstract. In this talk, I will describe our work on transfer learning for text and wireless sensor network data mining. Transfer learning allows the training and test data to come from different distributions. This research field is motivated by the practical need of acquiring more training data when data are easily outdated and quality labeled data are scarce. I will describe the background, techniques and some applications of transfer learning in several data mining applications.

Optimal portfolios with a VaR constraint

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Abstract. In market risk management, it is widely accepted that Value-at-Risk (VaR) is a useful summary measure of market risks and an option to be used by regulators and large banks to set the requirement on capital reserves. In order to fulfill the requirement, a portfolio must be able to control the level of VaR. If the expected utility of wealth or consumption is maximized over a certain period of time without considering risks, the optimal allocation to the risky asset might violate the VaR restriction at some points and fall short of the regulatory requirement. In this article, we impose the VaR as a dynamic constraint to the optimal portfolio problem. At each instant, the VaR is estimated and is applied to influence the investment decision. The optimal portfolio problem is formulated as a constrained maximization of the expected utility, with the constraint being the VaR level. Dynamic programming is applied to reduce the whole problem to solving the Hamilton-Jacobi-Bellman equation coupled with the VaR constraint, and the method of Lagrange multiplier is then applied to handle the constraint. A numerical method is proposed to solve the problem. By applying the VaR constraint continuously over time, we find that investments in risky assets are reduced whenever the VaR constraint becomes active.

A group of knowledge-incorporated multiple criteria linear programming classifier

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Abstract. Multiple Criteria Linear Programming (MCLP) is used as a classification method, which can separate two or more classes by finding discriminate hyperplane. When facing with nonlinear separable data, MCLP is no longer applicable. Kernel-based Multiple Criteria Linear Programming (KMCLP) model is developed to solve nonlinear separable problem. In this method, kernel function is introduced to project the data into a higher-dimensional space in which the data will have more chance to be linear separable. KMCLP performs well in some real applications. However, just as other prevalent data mining classifiers, MCLP and KMCLP learn only from training examples. In traditional machine learning area, there are also classification tasks in which data sets are classified only by prior knowledge, i.e. expert system. Some works combine the above two classification principle to overcome the defaults of each approach. In this paper, we summarize the relevant works which combine the prior knowledge and MCLP or KMCLP model to solve the problem when input consists of not only training example, but also prior knowledge. Specifically, knowledge-incorporated MCLP model deals with linear knowledge and linear separable classification problem. The prior knowledge in the form of polyhedral knowledge sets can be expressed into logical implications, which can further be converted into a series of equalities and inequalities. Incorporating such kind of constraints to original MCLP model, we then obtain the final knowledge-incorporated MCLP model. Linear knowledge can also be introduced into kernel-based MCLP model by transforming the logical implication into the expression with kernel. With this approach, nonlinear separable data with linear knowledge can be easily classified. Concerning the nonlinear prior knowledge, by writing the knowledge into logical expression, the nonlinear knowledge can be added as constraints to the kernel-based MCLP model. It then helps to find the best discriminate hyperplane of the two classes. Numerical tests on the above models indicate that they are effective in classifying data with prior knowledge.

Mining labeled and unlabeled data via multiple criteria linear programming classification model

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Abstract. In business data mining, it is always expensive to get labeled exam- ples. A common situation is that a training sample with a few labeled examples and a lot unlabeled examples is used to build model, which raises new chanlleges to many traditional supervised learning models such as the Multiple Criteria mathematical Programming (MCMP) classification models. Recently, these MCMP models have been widely used in classification and gradually formulated as a new family in data mining. A well-known member of this MCMP family is the Multiple Criteria Linear Programming (MCLP) model. Although MCLP, as many works have shown, can build a satisfactory model only with the labeled data, it can not use the information behind the unlabled examples which are assumed to provide additional distribution information of the training sample. To overcome this shortage, in this paper, we present a new Semi-Supervised Multiple Criteria Linear Programming (S^2MCLP) model which builds model from both labeled and unlabeled data.

Consider a problem of binary classification. The training set D consists of l labeled examples $\{(x_i, y_i)\}_{i=1}^{l}$, $y_i = \{-1, 1\}$, and u labeled examples $\{x_i\}_{i=l+1}^{n}$ with $n = l + u$. The original MCLP model tries to find a classification boundary b to maximize distances of the sum of the correct classified instances and minimize the distances of the sum of the misclassified instances simultaneously. By using the linear combination of these two objective functions, MCLP solves the following optimization problem

(Model 1: original MCLP Model)

$$\begin{aligned} &minimize \ \sum_{i=1}^{l} \alpha_i - w \sum_{i=1}^{l} \beta_i \\ &subjectto: \\ &A_i X - \alpha_i + \beta_i = b, A_i \in -1 \\ &A_i X + \alpha_i - \beta_i = b, A_i \in +1 \end{aligned} \tag{1}$$

where A_i are the labeled instances, x and b are unrestricted, α_i, $\beta_i \geq 0$. b is the classification boundary.

In original MCLP model (1), the constrains are separated into two different formulations according to which groups Ai belongs to. To simplify this formulation, we put the label value y into the constrains and transform Model (1) into a much succinct one as follows:

(Moel 2: Succinct MCLP Model)

$$\begin{aligned} &minimize \ \sum_{i=1}^{l} \alpha_i - w \sum_{i=1}^{l} \beta_i \\ &subjectto: \\ &A_i X - b = y_i(\beta_i - \alpha_i), \quad 1 \leq i \leq l \end{aligned} \tag{2}$$

where A_i are the labeled instances, x and b are unrestricted, α_i, $\beta_i \geq 0$. b is the classification boundary.

As we discussed above, Model (2) is a supervised learning model which can only learn from the labeled instances. To learn from the unlabeled instances, we should introduce two assumptions first: (1) cluster assumption: the classification boundary is more likely to traverses through low data density regions, in other words, instances in a data cluster probably have the same labels; (2)although the class labels of the unlabeled data are not known a prior, we believe that maximizing the distance between the instance x_i and the boundary b can help to identify the genuine classification surface. Thus, for each unlabeled instance x_i, we should maximize the distances of $|A_i x - b|$. According to the constrain $A_i X - b = y_i(\beta_i - \alpha_i)$, maximizing $|A_i x - b|$ is equivalent to maximizing $|y_i(\beta_i - \alpha_i)| = \beta_i - \alpha_i$ Thus the Semi-Supervised MCLP model can be formulated as follows:

(Moel 3: S^{2}MCLP Model)

$$
\begin{aligned}
&minimize \ \sum_{i=1}^{l}(\alpha_i - w\beta_i) - C^* \sum_{i=l}^{l+u} |\alpha_i - \beta_i| \qquad (3)\\
&subjectto:\\
&A_i X - b = y_i(\beta_i - \alpha_i), \quad 1 \leq i \leq l\\
&A_i X - b = |\beta_i - \alpha_i|, \quad l \leq i \leq l+u
\end{aligned}
$$

where A_i are the training instances, x and b are unrestricted, α_i, $\beta_i \geq 0$. b is the classification boundary.

A new multiple criteria programming approach based on rough approximation for classification

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Abstract. This paper puts forward a new and effective approach based on rough set and multiple criteria programming (MCP) for solving classification problems in data mining. Firstly, we describe the basic theories of rough set and set approximation. Then we provide the methodology and model of the multiple criteria programming approach based on rough approximation for classification, which sufficiently use the basic ideas of rough set and the principles of MCP approach. In addition, we also develop and implement the algorithm in SAS system and Windows platform. Finally, conclusions and comparison analysis of many experiments in practical data set and related applications show that this classification approach is better than ordinary MCP model and other traditional classification methods in classification accuracy rate and efficiency.

A novel classification method based on l_1 norm distance

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Abstract. This paper proposes a novel pattern classification approach, called l_1 norm nearest neighbor convex hull (l_1 NNCH) method for data classification. As we all know, the single nearest neighbor (1-NN) classifier is often used for classification, which is a most intuitive approach based on the nearest neighbor rule. In 1-NN, a query is decided to the class including the nearest prototype to it. 1-NN relies crucially on the assumption that training samples are representative of the query. Its classification results depend on how training samples are chosen to account for possible sample variations and also how many training samples are available. However, in general only a finite number of training samples are available. Accounting for more samples changes than the original samples, l_1 NNCH method uses the convex hull of each class training samples to expand the representational capacity of the training set. A convex hull of a class samples is the smallest convex polytope covering that set, which provides an infinite number of unseen training points to represent the query. Moreover, in l_1 NNCH approach, l_1 norm distance is also adopted to define similarity measurement for classification. As an important distance measure, l_1 norm is widely used in pattern classification. l_1 NNCH approach defines l_1 norm distance from a query to a convex hull of a class as the similarity of the nearest neighbor rule, and then the query is classified into the class with minimal l_1 norm convex hull distance. Experimental results on the ORL and NJUST603 face database show that l_1 NNCH approach has a good classification performance.