WORKSHOP ON

Computational Mathematics

21 – 22 December 2006

S14, #03-10

Department of Mathematics

National University of Singapore

A JOINT EVENT BY

PROGRAMME
Thursday, 21 December 2006

Chair: Zhu Chengbo, NUS

09:05 - 09:20 Opening Ceremony

Welcome address by Tan Eng Chye, Dean, Faculty of Science, NUS

Speech by Han Danfu, Deputy Head, Department of Mathematics, Zhejiang University

09:20 - 10:00 Wavelets: Some New Developments

Lee Seng Luan, NUS

10:00 - 10:40 Online and Offline Algorithms for Two-Dimensional Knapsack

Zhang Guochuan, Zhejiang University

10:40 - 11:10 Break

Chair: Lin Ping, NUS

11:10 - 11:50 An Introduction to Bivariate Spline Method for Numerical Solution of PDEs and Scattered Data Fitting

Han Danfu, Zhejiang University

11:50 - 14:00 Lunch

Chair: Sun Defeng, NUS

14:00 - 14:40 An Inexact Primal-Dual Path Following Algorithm for Convex Quadratic SDP

Toh Kim Chuan, NUS

14:40 - 15:20 Constraint Qualifications for Convex Inequality Systems with Applications in Constrained Optimizations

Li Chong, Zhejiang University

15:20 - 15:50 Break

Chair: Li Chong, Zhejiang University

15:50 - 16:30 Combinatorial Constructions for Optimal Frequency-Hopping Sequences

Ge Gennian, Zhejiang University

16:30 - 17:10 A Dual Optimization Approach for Inverse Quadratic Eigenvalue Problems with Partial Eigenstructure

Sun Defeng, NUS

PROGRAMME
Friday, 22 December 2006

Chair: Zhu Jianxin, Zhejiang University

09:00 - 09:4 Iterative Method for Planar Linear Elasticity Problem with Large Lame Constant
Chen Xiaoliang, Zhejiang University

09:40 - 10:20 Numerical Simulation for Rotating Bose-Einstein Condensates
Bao Weizhu, NUS

10:20 - 10:50 Break

Chair: Bao Weizhu, NUS

10:50 - 11:30 Finite Element Methods for Molecule Orientations of Liquid Crystals and Liquid Crystal Flows
Lin Ping, NUS

11:30 - 12:10 Leaky Modes and Berenger's Modes of Slab Waveguides - Asymptotic Solutions
Zhu Jianxin, Zhejiang University

12:10 - 14:00 Lunch

Chair: Jin Hanqing, NUS

14:00 - 14:40 The Numerical Computation of Hamiltonian Schur Form
Chu Delin, NUS

14:40 - 15:20 On the Local Convergence of Several Iterations
Huang Zhengda, Zhejiang University

15:20 - 15:50 Break

Chair: Huang Zhengda, Zhejiang University

15:50 - 16:30 Numerical Methods for Total Variation Minimization Problems
Andy Yip Ming Ham, NUS

1630 - 17:10 Portfolio Selection with Ambiguity
Jin Hanqing, NUS

ABSTRACTS

Wavelets: Some New Developments

Lee Seng Luan
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In the past two decades, wavelets and frames have proved to be useful in image processing. Recent development in geometric modelling, computer graphics, visualization and numerical approximations have motivated the construction of wavelets and frames based on other multiscale and multiresolution information, such as discrete geometry information generated by subdivision processes and discrete functional data generated by other numerical methods. This talk gives some recent developments of wavelets in this direction.

Online and Offline Algorithms for Two-Dimensional Knapsack

Zhang Guochuan
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Given a set of rectangles, each of which is associated with a profit, we are requested to pack a subset of the rectangles into a bigger rectangle (knapsack) so that the total profit of rectangles packed is maximized. The rectangles may not overlap. This problem is strongly NP-hard even for packing squares with identical profits into a square bin. We will present several (offline) approximation algorithms for the general case and some special cases that the rectangles are of the same profit and that the profit of a rectangle is equal to its area.

We further deal with the online version where the rectangles arrive one by one. To reach reasonable results a relaxed problem called online removable square packing is investigated. For a sequence of squares with side length at most 1, we are requested to pack a subset of them into a unit square (knapsack) where the online player can decide whether to take the current square or not and which squares currently in the unit square to remove. The goal is to maximize the total area of rectangles packed into the knapsack. Competitive online algorithms are devised.

This talk is based on joint work with X. Han, K. Iwama and K. Jansen.

ABSTRACTS

An Introduction to Bivariate Spline Method for Numerical Solution of PDEs and Scattered Data Fitting

Han Danfu
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Bivariate splines of various degrees over various triangles are considered in this talk. The matrix form of the smoothness conditions for these bivariate splines is presented. Upon this form, the spline method for numerical solution of partial differential equations has been extended to this spline space of various degrees. The generalized spline method has been implemented to solve PDE's with a singularity at the boundary. Numerical examples show the effectiveness of the generalized spline method. Meanwhile, for given a set of scattered data with derivatives values, Hermite interpolation based on bivariate spline spaces over triangulation is also considered by minimal energy method.

An Inexact Primal-Dual Path Following Algorithm for Convex Quadratic SDP

Toh Kim Chuan
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We propose interior-point (IP) methods for linearly constrained convex quadratic semidefinite programming.

At each IP iteration, the search direction is computed from an m+n(n+1)/2 dense augmented system, which only be solved by iterative methods when n > 100. We propose three classes of preconditioners for the augmented matrix.
The preconditioned matrices have favorable asymptotic spectra under suitable assumptions.

Numerical results show that our methods are efficient and robust

Constraint Qualifications for Convex Inequality Systems with Applications in Constrained Optimizations

Li Chong
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For an inequality system defined by an infinite family of proper convex functions, we study the basic constraint qualification and other conditions defined by the epigraphs of the conjugate functions of these functions. Several sufficient conditions ensuring the BSQ are provided. Applications are discussed in the areas of conic programming, constraint optimization and approximation theory.

ABSTRACTS

Combinatorial Constructions for Optimal Frequency-Hopping Sequences

Ge Gennian
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Frequency-hopping multiple-access (FHMA) spread-spectrum communication systems employing multiple frequency shift keying as data modulation technique were investigated by Fuji-Hara, Miao and Mishima [R. Fuji-Hara, Y. Miao and M. Mishima, *Optimal frequency hopping sequences: a combinatorial approach*, IEEE Trans. Inform. Theory, **50** (2004), 2408--2420] from a combinatorial approach, where a correspondence between frequency-hopping (FH) sequences and partition-type cyclic difference packings was established, and several combinatorial constructions were provided for FHMA systems with a single optimal FH sequence. In this talk, by means of this correspondence, we describe more combinatorial constructions for such optimal FH sequences. As a consequence, more new infinite series of optimal FH sequences are obtained.

A Dual Optimization Approach for Inverse Quadratic Eigenvalue Problems with Partial Eigenstructure

Sun Defeng
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The inverse quadratic eigenvalue problem (IQEP) arises in the field of structural dynamics. It aims to find three symmetric matrices, known as the mass, the damping and the stiffness matrices, respectively such that they are closest to the given analytical matrices and satisfy the measured data. The difficulty of this problem lies in the fact that in applications the mass matrix should be positive definite and the stiffness matrix positive semidefinite. Based on an equivalent dual optimization version of the IQEP, we present a quadratically convergent Newton-type method. Our numerical experiments confirm the high efficiency of the proposed method.

Iterative Method for Planar Linear Elasticity Problem with Large Lame Constant

Chen Xiaoliang
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In this talk, we propose an iterative algorithm for planar linear elasticity problem with large Lame constant. We prove the algorithm convergent uniformly with the large Lame constant. We overcome the inf-sup condition and we can use the linear or bilinear element. We will also give some remarks of the algorithm to solving the Reissner-Mindlin plate problem.

ABSTRACTS

Numerical Simulation for Rotating Bose-Einstein Condensates

Bao Weizhu
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In this talk, we present efficient and stable numerical methods to compute ground states and dynamics of Bose-Einstein condensates (BEC) in a rotational frame. As preparatory steps, we take the 3D Gross-Pitaevskii equation (GPE) with an angular momentum rotation, scale it to obtain a four-parameter model and show how to reduce it to 2D GPE in certain limiting regimes. Then we study numerically and asymptotically the ground states, excited states and quantized vortex states as well as their energy and chemical potential diagram in rotating BEC. Some very interesting numerical results are observed. Finally, we study numerically stability and interaction of quantized vortices in rotating BEC. Some interesting interaction patterns will be reported.
Mindlin plate problem.

Finite Element Methods for Molecule Orientations of Liquid Crystals and Liquid Crystal Flows

Lin Ping
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The liquid crystal molecule orientation is arranged by minimizing so-called Oseen-Frank energy functional. The energy is nonconvex due to the unit-length constraint of liquid crystal molecules and the constraint is treated by the penalty method. A pseudo-Newton method with a multi-grid linear system solver or preconditioner is used to compute the solution. Due to small parameters in the model and singularities in the solution a homotopy algorithm combined with a mesh refinement strategy (based on a posteriori error estimate) is found to be very robust for both 2D and 3D simulations. The liquid crystal flow is a coupling between a director field (molecule orientation) of liquid crystals and a flow field. The model is also related to phase field models of multiphase flows and to microfluidics device. It is crucial to preserve the energy law of the system in numerical simulation, especially when orientation singularities are involved. We present a discrete energy preserving C0 finite element method. It is of second order and matrix free in time. A number of liquid crystal flow examples (including small and large molecule cases) are computed to demonstrate the algorithm.

ABSTRACTS

Leaky Modes and Berenger's Modes of Slab Waveguides - Asymptotic Solutions

Zhu Jianxin
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Approximate analytic solutions of the leaky modes and Berenger's modes in two-dimensional slab waveguides are derived through an asymptotic analysis. General slab waveguides with ghree layers of possibly different refractive indexes are studied for both the transvers electric (TE) and transverse magnetic ™ cases. The results are useful in the eigenmode expansion method, where the leaky modes and Berenger's modes appear if a perfectly matched layer (PML) is used to terminate the transverse directions of optical waveguides.

The Numerical Computation of Hamiltonian Schur Form

Chu Delin
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In this talk we will introduce a new numerical method for computing the Hamiltonian Schur for of a 2n-by-2n Hamiltonian matrix. The properties of the new methods are demonstrated by showing its performance for the Benchmark collection of continuous-time algebraic Riccati equations.

On The Local Convergence of Several Iterations

Huang Zhengda
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Let

$$f(x) = 0, \tag{1}$$

where $f : D \subset E \to F$ is an nonlinear operator defined on the convex set D of Banach spaces E and valued in same type space F.

We are going to study the local convergence of methods in Euler family defined by

$$x_{n+1} = G^n_{k,f}(x), \quad x \in D, \quad n \geq 1, \tag{2}$$

and a family of iterations with parameter α for solving nonlinear equation (1) defined by

$$x_{n+1,\alpha} = HE^n_{f,\alpha}(x_{0,\alpha}), \quad x_{0,\alpha} \in D, \quad n \geq 1, \tag{3}$$

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where

$$G_{k,f}(x) = x + \sum_{i=1}^{k} \frac{1}{i!}[f_x^{-1}(f(x))]^{(i)}(-f(x))^i,$$

and

$$HE_{f,\alpha}(x) = x - [I + \frac{1}{2}[I - \alpha L_f(x)]^{-1} L_f(x))f'^{-1}(x)f(x), \qquad x \in D,$$

$\alpha \in (-\infty, +\infty)$, and

$$L_f(x) = f'(x)^{-1} f''(x) f'(x)^{-1} f(x), \qquad x \in D.$$

Under kinds of generalized Lipschitz conditions, we get the crucial radius of convergent ball of methods of (2) and of (3) with $\alpha \leq 0$.

For (2), we show that the local convergence of the method is guaranteed by a period 2 orbit in R or by a repelling additional fixed point of the method. Also the radius of convergent balls of methods decreases as k increases.

For (3), we get that the local convergence of (3) with $\alpha \leq 0$ is guaranteed by a repelling additional fixed point in C, and that the convergence ball of $\alpha > 0$ is no more less than the ball of $\alpha \leq 0$.

Numerical Methods for Total Variation Minimization Problems

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Total variation regularization has been successfully applied various image restoration problems such as denoising, deblurring, inpainting and segmentation. The main advantage is that it preserves edges which are important features for visual perception. However, due to the non-linearity and non-differentiablility of the total variation norm, it is non-trivial to minimize total variation efficiently. In this talk, I will present some recent numerical methods for total variation minimization.

Portfolio Selection with Ambiguity

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In a financial market, the appreciate rates of risky assets are statistically very difficult to estimate precisely, and usually only some confidence interval will be estimated. This work is devoted to the portfolio selection with the appreciation rates being in a certain convex set rather than being specified precisely. We study the problem in both expected utility framework and mean-variance framework, and robust solutions are given explicitly in both frameworks.