WORKSHOP ON

Computational Mathematics

21 - 22 December 2006
S14, #03-10
Department of Mathematics
National University of Singapore

A JOINT EVENT BY

NUS
National University of Singapore

ZHEJIANG UNIVERSITY
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

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 - 09:40 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
16:30 - 17:10 Portfolio Selection with Ambiguity
   Jin Hanqing, NUS
Wavelets: Some New Developments

Lee Seng Luan  
Department of Mathematics, National University of Singapore  
Email: matleesl@nus.edu.sg

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  
Department of Mathematics, Zhejiang University  
Email: zgc@zju.edu.cn

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

Han Danfu
Department of Mathematics, Zhejiang University
Email: mhdf2@zju.edu.cn

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
Department of Mathematics, National University of Singapore
Email: mattohkc@nus.edu.sg

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
Department of Mathematics, Zhejiang University
Email: cli@zju.edu.cn

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.
Combinatorial Constructions for Optimal Frequency-Hopping Sequences

Ge Gennian
Department of Mathematics, Zhejiang University
Email: gnge@zju.edu.cn

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
Department of Mathematics, National University of Singapore
Email: matsundf@nus.edu.sg

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
Department of Mathematics, Zhejiang University
Email: xiaoliangcheng@zju.edu.cn

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.
**Numerical Simulation for Rotating Bose-Einstein Condensates**

**Bao Weizhu**  
Department of Mathematics, National University of Singapore  
Email: bao@math.nus.edu.sg

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.

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

**Lin Ping**  
Department of Mathematics, National University of Singapore  
Email: matlinp@nus.edu.sg

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.
Leaky Modes and Berenger’s Modes of Slab Waveguides - Asymptotic Solutions

Zhu Jianxin
Department of Mathematics, Zhejiang University
Email: zjxmath@163.com

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 three layers of possibly different refractive indexes are studied for both the transvers electric (TE) and transverse magnetic (TM) 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
Department of Mathematics, National University of Singapore
Email: matchudl@nus.edu.sg

In this talk we will introduce a new numerical method for computing the Hamiltonian Schur form 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
Department of Mathematics, Zhejiang University
Email: zdhuang@css.zju.edu.cn

Let

\[ f(x) = 0, \]

where \( f : D \subseteq E \to F \) is a nonlinear operator defined on the convex set \( D \) of Banach spaces \( E \) and valued in some type space \( F \).

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

\[ x_{n+1} = G_{R,f}(x), \quad x \in D, \quad n \geq 1, \]

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

\[ x_{n+1,\alpha} = H\mathcal{E}_{P,f,\alpha}(x_{0,\alpha}), \quad x_{0,\alpha} \in D, \quad n \geq 1, \]
where
\[ G_{k,f}(x) = x + \frac{1}{k} \sum_{i=1}^{k} [-f_x^{-1}(f(x))]^i (-f(x))^i, \]
and
\[ H_{E,f,\alpha}(x) = x - [I + \frac{1}{2} [I - \alpha L_f(x)]^{-1} L_f(x)] f^{-1}(x) f(x), \quad x \in D, \]
\[ \alpha \in (-\infty, +\infty), \text{ and} \]
\[ L_f(x) = f'(x)^{-1} f''(x) f'(x)^{-1} f(x), \quad x \in D. \]

Under some 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 than the ball of \( \alpha \leq 0 \).

**Numerical Methods for Total Variation Minimization Problems**

**Andy Yip Ming Ham**

Department of Mathematics, National University of Singapore  
Email: matymha@nus.edu.sg

Total variation regularization has been successfully applied various image restoration problems such as denoising, deburring, 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-differentiability 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**

**Jin Hanqing**

Department of Mathematics, National University of Singapore  
Email: matjinh@nus.edu.sg

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 appreciate 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.