Canada-China-USA Conference on

Modern Techniques in Computational Mathematics

August 22-24, 2011

Invited Speakers

Liqun Cao, Chinese Academy of Sciences, China
Raymond H. Chan, The Chinese University of Hong Kong, China
Qianshun Chang, Chinese Academy of Sciences, China
Feng Dai, University of Alberta, Canada
Jeff Geronimo, Georgia Institute of Technology, USA
Bin Han, University of Alberta, Canada
Don Hong, Middle Tennessee State University, USA
Rong-Qing Jia, University of Alberta, Canada
Song-Tao Liu, Morgan Stanley, New York, USA
Bradley J. Lucier, Purdue University, USA
Qun Mo, Zhejiang University, China
Lixin Shen, Syracuse University, USA
J. Derek Tucker, Naval Surface Warfare Center, USA
Jianzhong Wang, Sam Houston State University, USA
J. D. Ward, Texas A&M University, USA
Yau Shu Wong, University of Alberta, Canada
Yuesheng Xu, Syracuse University, USA (and Guangdong Province Key Laboratory of Computational Science, and Sun Yet-sen University, China)
Zhiqiang Xu, Chinese Academy of Sciences, China
Wei Zhao, McMaster University, Canada
Jiang Zhu, National Laboratory for Scientific Computing-LNCC, Brazil

University of Alberta
Edmonton
Canada

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The main objective of this conference is to bring together leading experts in computational mathematics from Canada, China, and USA. The conference will provide a forum to review recent advancements and to investigate future developments of modern techniques in computational mathematics. The emphasis of the conference will be placed on the following topics:

- The techniques of optimization for variational models of image processing
- The techniques of multigrids and wavelets for numerical pde's
- Wavelets and framelets and their applications
- Multivariate approximation on spheres and manifolds
- Random matrices and compressive sampling
- Statistical analysis and learning theory
- Applications to financial mathematics
- Applications to medical sciences

Sponsors

The conference is supported by the following organizations and institutions:

- Natural Sciences and Engineering Research Council of Canada
- the China Institute, Department of Mathematical and Statistical Sciences and the Applied Mathematics Institute of University of Alberta
- Pacific Institute of Mathematical Sciences (PIMS)

Organization Committee

The conference is organized by Rong-Qing Jia and Yau Shu Wong.

Venue

All the presentations take place in Room 235, CAB (Central Academic Building).

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University of Alberta, Edmonton, Canada
Central Academic Building, Room 235

Program

Morning Session, August 22 Chairman: Rong-Qing Jia

8:30–9:20: *Raymond H. Chan*
Framelet-Based Algorithm for Medical Imaging Applications

9:20–10:10: *Bradley J. Lucier*
Multiscale Besov Space Smoothing of Images

10:30–11:20: *Yuesheng Xu*
Proximity Fixed-Point Algorithms for Image Denoising

11:20–12:10: *Lixin Shen*
A Study on the L1/TV Model

Afternoon Session, August 22 Chairman: Jianzhong Wang

2:00–2:50: *Jeff Geronimo*
Intertwining Multiresolution Analysis and the Construction of Bivariate Compactly Supported Continuous Orthogonal Piecewise Polynomial Scaling Functions and Wavelets

2:50–3:40: *Bin Han*
Wavelets and Framelets in Function Spaces

4:00–4:50: *Don Hong*
Computational Statistical Applications to Imaging Mass Spectrometry Based Proteomic Data Analysis and Biomarkers Discovery

4:50–5:40: *Wei Zhao*
Mathematical Modeling and Multilevel Computation of Dispersed Drug Release from Swellable and Erodible Polymeric Matrix Systems

Morning Session, August 23, 2011 Chairman: Bin Han

8:30–9:20: *Yau Shu Wong*
Exact Finite Difference Schemes for Solving Helmholtz Equation at Any Wavenumber

9:20–10:10: *J. Derek Tucker*
Statistical Analysis and Modeling of Elastic Functions

10:30–11:20: *Liqun Cao*
Multiscale Computation and Analysis for Schrödinger-Poisson System in Heterogeneous Materials

11:20–12:10: *Jiang Zhu*
Finite Element Methods for Nonlinear Coupled Problems

Afternoon Session, August 23, 2011 Chairman: J. D. Ward

2:20–3:10: *Qianshun Chang*
Several Fast Algorithms of Split Bregman Method and Comparisons for Deblurring and Denoising

3:10–4:00: *Jianzhong Wang*
Randomized Approximation of the Feature Vectors of Large-size Reproducing Kernels

4:20–5:10: *Rong-Qing Jia*
Applications of the Uzawa Algorithm to Numerical PDE's, Compressive Sampling and Image Processing

5:10–6:00: *Song-Tao Liu*
Numerical Methods for Financial Mathematics

Morning Session, August 24, 2011 Chairman: Yau Shu Wong

8:30–9:20: *J. D. Ward*
Kernel-based Interpolation and Approximation on Manifolds

9:20–10:10: *Feng Dai*
Moduli of Smoothness on the Unit Ball

10:30–11:20: *Zhiqiang Xu*
The Error Bound for PCM Quantization

11:20–12:10: *Qun Mo*
Some New Bounds of the R.I.C. in Compressed Sensing

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Abstracts

Multiscale Computation and Analysis for Schrödinger-Poisson System in Heterogeneous Materials

Liqun Cao
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In this talk, we discuss the multiscale computation for Schrödinger-Poisson system arising from the electronic properties of semiconductors such as quantum wells, wires and dots, and CMOS transistor. We first introduce the Schrödinger equations with the effective mass approximation which has been particularly successful in the case of heterostructures. Combining Allaire's work and our result, we give an interpretation why the effective mass approximation is very successful for calculating the band structures of semiconductor nanostructures in the vicinity of Γ point, from the viewpoint of mathematics. Second, we analyze the relationship between microscopic Maxwell's equations and macroscopic Maxwell's equations. Furthermore, we discuss mathematical modeling of electromagnetics at nano-scale and offer an explanation as to why Schrödinger-Poisson equations and Maxwell-Schrödinger equations have been widely used to semiconductor nanostructures. Third, the multiscale method for Schrödinger-Poisson system in heterogeneous materials is presented. Numerical simulations are carried out to validate the theoretical results. Finally, some unsolved problems are advanced.

Framelet-Based Algorithm for Medical Imaging Applications

Raymond H. Chan
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Framelets have been used successfully in various problems in image processing, including inpainting, impulse noise removal, super-resolution image restoration, etc. In this talk, we will introduce two new applications of the tight-frame algorithm in medical imaging. The first one is segmentation which is the process of identifying object outlines within images. We apply the framelet-based approach to identify tube-like structures such as blood vessels in magnetic resonance angiography images. Our method iteratively refines a region that encloses the possible boundary or surface of the vessels. Results on real 2D/3D images demonstrate that the method is very efficient and outperforms other existing methods. The second application is image reconstruction for parallel magnetic resonance imaging (MRI).

Parallel MRI plays a very important role in reducing the image acquisition time, but often the restored image suffers from reconstruction artifacts such as aliasing. We apply tight-frame algorithm to iteratively reconstruct the desired image while eliminating the artifacts. Results on phantom and real MRI images show that our method outperforms standard package such as SENSE in terms of robustness to both noise and the estimation of coil sensitivities.

Several Fast Algorithms of Split Bregman Method and Comparisons for Deblurring and Denoising

Qianshun Chang
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The split Bregmanmethod is an efficient algorithm for denoising and deblurring. In the split Bregman method, only a linear system of equations is implicit and needs to solve.

In this talk, we discuss implementation of the split Bregman method. Mainly, we propose several fast algorithms for solving the system in the split Bregman method. i) The system is solved by the algebraic multigrid method and the inner iteration is accelerated by Krylov subspace method. ii) A splitting scheme of alternative one-dimension is applied to solve the system. iii) The FFT method is directly applied to solve the system. iv) Using Neumann boundary condition for the blur operator, the FFT method is applied to solve the system.

As comparison, the fast TV method (Y. Huang, M. K. Ng and Y. Wen, A fast total variation minimization method for image restoration, SIAM J. Multiscale Model Simul., 7 (2008) pp. 774–795) is discussed in this talk.

The results of numerical experiments are given and compared. At last, some discussion and remark on these methods are given.

Moduli of Smoothness on the Unit Ball

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This is a joint work with Yuan Xu (University of Oregon). A class of differential operators are discussed in connection with the orthogonal polynomial expansions on the unit ball. A new K-functional using these differential operators is defined on the unit ball, and is shown to be equivalent to a new modulus of smoothness, which satisfies all the usual characteristic properties of moduli of smoothness, including direct and inverse theorems for best polynomial approximation. Moreover, our modulus of smoothness on the unit ball is computable, and is new even in the case of one variable. Finally, an analogue of the Ditzian-Totik modulus of smoothness is introduced on the unit ball, and is studied in connection with our new modulus.

Intertwining Multiresolution Analysis and the construction of bivariate compactly supported continuous orthogonal piecewise polynomial scaling functions and wavelets

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We will review the technique of intertwining multiresolution analysis and apply it to construct compactly supported orthogonal, continuous, bivariate, piecewise polynomial wavelets supported on squares and hexagons. This is work with George Donovan and Doug Hardin.

Wavelets and Framelets in Function Spaces

Bin Han
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In this talk, we shall present some recent results on wavelets and framelets in function spaces such as Sobolev and Besov spaces, which are of particular interest in many wavelet-based applications. We shall present the basic theory on wavelets and framelets in function spaces. Then we discuss some general results about deriving wavelets and framelets in function spaces from refinable functions. Examples will be provided to illustrate the general theory. If time permits, we will also present some theoretical results on frequency-based framelets and directional tight framelets.

Computational Statistical Applications to Imaging Mass Spectrometry Based Proteomic Data Analysis and Biomarkers Discovery

Don Hong
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In proteomics study, Imaging Mass Spectrometry (IMS) is an emerging and very promising new technique for protein analysis from intact biological tissues. Though it has shown great potential for rapid mapping of protein localization and the detection of sizeable differences in protein expression, challenges remain in data processing due to the difficulty of high dimensionality and the fact that the number of variables chosen to be used in prediction model is significantly larger than the number of observations.

To obtain a complete overview of IMS data and find trace features based on both spectral and spatial patterns, one faces a global optimization problem. In this talk, some recent progress on the IMS data processing will be presented including the multivariate analysis and statistical learning applications to IMS cancer data analysis and the development of a new software package called IMSmining using both spectral and spatial information for biomarker selection of IMS data. Experimental data analysis results show that IMSmining produces more concise peak list, confirms new biomarkers, and provides better classification rate.

Applications of the Uzawa Algorithm to Numerical PDE's, Compressive Sampling and Image Processing

Rong-Qing Jia
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In this talk we will discuss applications of the Uzawa algorithm to numerical solutions of partial differential equations, compressive sampling and image processing. We indicate that many apparently different algorithms can be viewed as variations of the Uzawa algorithm. We also design some explicit iteration algorithms and establish convergence of the iteration independent of the step size. Finally, we will address the difficult question of convergence rates of the iteration scheme.

Numerical Methods for Financial Mathematics

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In this talk, we will discuss two numerical methods used for some financial mathematics problems: Fourier transform methods and PDEs by alternative direction implicit finite difference methods. We will also explore the possibility of multi-grid and wavelet preconditioning methods for solving two dimensional evolution PDEs in finance.

Multiscale Besov Space Smoothing of Images

Bradley J. Lucier
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We consider a variant of Rudin–Osher–Fatemi variational image smoothing that replaces the BV semi-norm in the penalty term with the $B^1_\infty(L_1)$ Besov space semi-norm. The space $B^1_\infty(L_1)$ differs from BV in a number of ways: It is somewhat larger than BV, so functions in $B^1_\infty(L_1)$ can exhibit more general singularities than exhibited by functions in BV, and, in contrast to BV, affine functions are assigned no penalty in $B^1_\infty(L_1)$. We provide a discrete model that uses a result of Ditzian and Ivanov to compute reliably with moduli of smoothness; we also incorporate some "geometrical" considerations into this model. We then present a convergent iterative method for solving the discrete variational problem. The resulting algorithms are multiscale, in that as the amount of smoothing increases, the results are computed using differences over increasingly large pixel distances. Some computational results will be presented. This is joint work with Greg Buzzard, Antonin Chambolle, and Stacey Levine.

Some New Bounds of the R.I.C. in Compressed Sensing

Qun Mo
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The restricted isometry constant is important in compressed sensing. In this talk, I shall report our recent results on some new bounds of the R.I.C.. First we shall give a new bound $\delta_{2s} < 0.4931$ as a sufficient condition for the ℓ_1-minimization problem to have a s-sparse solution. Next, we shall give a new bound $\delta_{s+1} < 1/(\sqrt{s}+1)$ as a sufficient condition for the orthogonal matching pursuit algorithm to recover each s-sparse signal in s iterations. Also, we shall use an example to show that bound is very tight. This example positively verifies the conjecture given by Dai and Milenkovic in 2009. These results are joint works with Song Li and Yi Shen.

A Study on the L1/TV Model

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In this talk, we will present our recent understanding on the L1/TV model. Based on different smoothing strategies, we will develop various algorithms for efficiently solving the model. The convergence of these algorithms will be discussed. The numerical experiments will demonstrate the efficiency of the algorithms.

Statistical Analysis and Modeling of Elastic Functions

J. Derek Tucker
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We introduce a novel geometric framework for separating, analyzing and modeling x (or horizontal) and the y (or vertical) variability in time-warped functional data of the type frequently studied in growth curve analysis and acoustic resonance structure. This framework is based on the use of the Fisher-Rao Riemannian metric that provides a proper distance for: (1) aligning, comparing and modeling functions and (2) analyzing the warping functions. A convenient square-root velocity function (SRVF) representation transforms the Fisher-Rao metric to the standard L_2 metric. It is applied to the given functions where it leads to a parametric family of penalized L_2 distances in SRVF space. These distances then are used to define Karcher means and the individual functions are optimally warped to align them to the Karcher means to extract their y variability. The resulting warping functions, which denote the x variability, are also analyzed using their own SRVFs thus transforming the manifold of such functions to a Hilbert sphere. Principal component analysis and stochastic modeling of these constituents (x and y) in their respective SRVF spaces leads to the desired modeling of functional variation. These ideas are demonstrated using both simulated and real data from sonar on proud targets providing a means for classification.

Randomized Approximation of the Feature Vectors of Large-size Reproducing Kernels

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In machine learning, compressive sensing, and high-dimensional data processing, reproducing kernels (which are also called diffusion kernels in data geometric harmonic analysis) play an important role. In most cases, several leading eigenvectors of such a kernel provide main features of the function to be learned, or the geometric properties of the data. However, in many application the kernel size is very large so that the classical eigen-decomposition methods become unpractical. Column based low-rank approximation for matrices, for example Nystrom approximation, is a wide-used technique. However, Nystrom approximation is subject to the column selection. It is hard to find a good scheme offering fast and effective selections. In this paper, we introduce a randomized algorithm for approximating the feature space, which has a very low-dimension. Applying classical eigen-decomposition methods on this space enable us to approximate the desirable feature vectors.

Kernel-based Interpolation and Approximation on Manifolds

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This talk will focus on kernel interpolation and approximation in a general setting. It turns out that for a wide class of compact, connected C^∞ Riemannian manifolds, including the important cases of spheres and $SO(3)$, the kernels obtained as fundamental solutions of certain partial differential operators generate Lagrange functions that are uniformly bounded and decay away from their center at a fast algebraic rate, and in certain cases, an exponential rate. This fact has important implications for both interpolation and approximation which will be discussed. The class of kernels considered in this talk include the restricted surface splines on spheres as well as surface splines for $SO(3)$, both of which have elementary closed form representations which are computationally implementable. The talk is based on some recent joint work with T. Hangelbroek and F.J. Narcowich along with previous work with the same co-authors together with X. Sun.

Exact Finite Difference Schemes for Solving Helmholtz Equation at Any Wavenumber

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The study of wave phenomena is important in many areas of science and engineering. The Helmholtz equation arises from time-harmonic wave propagation, and the solutions are frequently required in many applications such as aero-acoustic, underwater acoustics, electromagnetic wave scattering, and geophysical problems. Even though tremendous progress has been reported in the areas of computational techniques for partial differential equations, solving a linear Helmholtz equation at high wavenumbers numerically remains as one of the most difficult tasks in scientific computing. In this talk, we present novel difference schemes which do not introduce truncation error, and consequently the exact solution for the Helmholtz equation can be computed numerically at any wavenumbers. The power of this technique is illustrated by comparing numerical solutions for solving one- and two-dimensional Helmholtz equations using the standard second-order central finite difference and the proposed new finite difference schemes.

Proximity Fixed-Point Algorithms for Image Denoising

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We shall present the recent joint work with Micchelli and Shen on developing proximity fixed-point algorithms for solving the ROF image denoising model. The solution of the model will be characterized in terms of fixed-point equations, based on which fast algorithms will be developed. Connections of the proposed algorithms with the existing algorithms in the literature will be discussed. Numerical examples will be presented to demonstrate the accuracy and efficiency of the proposed algorithm.

The Error Bound for PCM quantization

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In signal processing, coding and many other practical applications, it is important to find a digital signal representation. Recently, the topic is very active in approximation theory. PCM scheme is a popular method to obtain the digital representation. In this talk, we will introduce the performance of the PCM scheme for quantizing finite unit-norm tight frame expansion without the White Noise Hypothesis. In particular, using results from number theory, we show that the up bound of PCM error is $\delta^{(d+1)/2}$. This is a joint work with Professor Yang Wang.

Mathematical Modeling and Multilevel Computation of Dispersed Drug Release from Swellable and Erodible Polymeric Matrix Systems

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Many drugs possessing low to mediate water solubility would experience gradual dissolution in modified release matrix systems. Thus drug release kinetics may be controlled by both dissolution and diffusion. A mathematical model of drug release from swellable and erodible matrix systems with initial drug loading higher than solubility was developed. The model was verified by the existing exact solution with the assumption of dissolution much faster than diffusion as a special case. Multilevel methods were introduced to solve the governing system of diffusion equations in order to achieve better approximation with lower computational costs. Finally, some further studies are proposed.

Finite Element Methods for Nonlinear Coupled Problems

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In this talk, a thermally coupled nonlinear elliptic system modeling a large class of engineering problems is considered. Some mathematical results are given first. Next, the C^0 Lagrangian finite element, the mixed finite element and the stabilized mixed DG approximations combined with a fixed point algorithm are proposed. Then the corresponding convergence analyses and error estimates are established, some numerical implementations are also presented. Finally, some further studies are proposed.